

DTIC FILE COPY

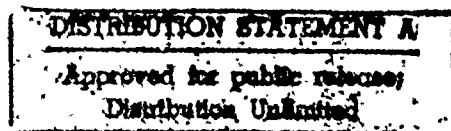
2

AD-A228 108

THE MARKET RESPONSES TO THE GOVERNMENT REGULATION
OF CHLORINATED SOLVENTS: A POLICY ANALYSIS

Thomas W. Chesnutt

October 1988



P-7548-RGS

90 10 26 057

The RAND Corporation

Papers are issued by The RAND Corporation as a service to its professional staff. Their purpose is to facilitate the exchange of ideas among those who share the author's research interests; Papers are not reports prepared in fulfillment of RAND's contracts or grants. Views expressed in a Paper are the author's own and are not necessarily shared by RAND or its research sponsors.

The RAND Corporation, 1700 Main Street, P.O. Box 2138, Santa Monica, CA 90406-2138

THE MARKET RESPONSES TO THE GOVERNMENT REGULATION
OF CHLORINATED SOLVENTS: A POLICY ANALYSIS

Thomas W. Chesnutt

PUBLICATION
DEPARTMENT

ERRATUM

P-7548-RGS *The Market Responses to the Government Regulation
of Chlorinated Solvents: A Policy Analysis*, by
Thomas W. Chesnutt, October 1988

Page i (title page)

The first full paragraph should read

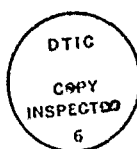
The original version of this study was prepared as a dissertation in October 1987 in partial fulfillment of the requirements of the doctoral degree in policy analysis at the RAND Graduate School. The faculty committee that supervised and approved the dissertation consisted of James Dertouzos (Chairman), Daniel Kohler, and Kathleen Wolf.

PREFACE

I would like to extend my appreciation to those who have contributed to this research. The list is short. The most important person in the formulative stages of this work was Dr. Kathleen Wolf who, by insisting on the primacy of chlorinated solvents in the life of any thinking person, managed to convince me of the importance of potentially toxic substances. Dr. Daniel Kohler deserves substantial credit for the genesis of the form of the empirical model. His continued advice and astute insight kept my modeling from plunging too far off into nihilistic jungles. Last, I put forth some of my very deepest thanks to Dr. James Dertouzos, the chair of the thesis committee, who drew me closer to an understanding of the meaning of Policy Analysis. I also forgive Jim for heeding the only words my father ever spoke to him: "Just don't be too easy on my boy."

I have other debts, intellectual and pecuniary, but I'll be unable to attribute all of them here. I do, however, hope to repay those I can within a reasonable period of time. My largest debts are to accounts I'll never be able to repay. Thanks.

The errors that remain are mine.



Accession For	
NTIS GRA&I	<input checked="checked" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By <i>per letter</i>	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
<i>A-1</i>	

SUMMARY

Under the Toxic Substances Control Act, the Environmental Protection Agency must oversee a wide range of chemicals that may harm humans or the environment. If each potentially toxic chemical were used completely independently of other potentially toxic chemicals, regulatory analysis of any chemical could ignore the effects of regulation upon other chemicals. If, as is the case, users of a chemical can substitute other chemicals, regulatory analysis must account for the second-order effects of regulation on the other chemicals.

This study argues that implicit risk tradeoffs among chemicals occur repeatedly as the response of economic markets to government regulation. It recommends, therefore, that such tradeoffs be formally incorporated into the analysis of regulatory alternatives.

Using publicly available historical data on chemical markets, the study builds a methodology to formally handle economic interrelationships among chemicals. The methodology can be used to analyze the effects of regulatory alternatives before the Environmental Protection Agency. (JS)

The case of markets for one set of functionally related chemicals--chemical solvents containing chlorine in their chemical structure--demonstrates the construction and application of an empirical model of related markets. The empirical model first measures the underlying economic forces in order to document the later effect of government regulation. The magnitude of government regulation, once documented, is then formally modeled and measured. Last, the model of interrelated markets is applied to demonstrate the system-wide effects of regulation on one or more chemicals.

The methodology bases the empirical analysis on a technical analysis. The construction of a model of economic relationships requires a sound understanding of the chemicals and their technical relationships. The technical knowledge, combined with the available data, ultimately drives the deterministic form of such a model.

The formal model of chlorinated solvent use links the use of a solvent to the levels of economic activity in various sectors of the economy that use the solvents. This deterministic form also includes sector-specific relative price measures to capture the effects of substitution among the solvents. A formal method to test for the endogeneity of the price measures shows the need to allow for the codetermination of price effects in a model of chlorinated solvent use.

The statistical estimation of the magnitude of the deterministic parameters, in turn, depends critically on the nondeterministic nature of the data. Account must be made for stochastic effects across chemical markets and through time. The deterministic and nondeterministic portions of the model of chlorinated solvent use are combined in the form of a series of steps to follow in the process of statistical estimation of model parameters.

The results of the estimation process applied to chlorinated solvent markets show the considerable effect of regulatory pressure on two chlorinated solvents: perchloroethylene and trichloroethylene. The models for markets of other chlorinated solvents that experienced a lower degree of regulatory pressure exhibit smaller effects in formal estimation. Among several alternatives for developing a proxy for the regulatory pressure on trichloroethylene, a flexible logistic proxy shows the most promise. Finally, an application of the chlorinated solvent use model evaluates the effect of regulation as an increase in the implicit cost of using the regulated chemical.

The historical approach, incorporating both a technical and an empirical analysis to examine the effect of regulation on markets for chlorinated solvents, demonstrates the implicit risk tradeoffs that occur when markets substitute among chemicals in the presence of regulation. In the future, the model may be used to analyze proposed regulatory alternatives.

CONTENTS

PREFACE	iii
SUMMARY	v
FIGURES	ix
TABLES	xi
Section	
I. INTRODUCTION	2
II. BACKGROUND	4
The Toxic Substances Control Act	4
Alternative Approaches	12
Market Response: The Approach	16
III. TECHNICAL ANALYSIS	17
History Of The Origin And Commercialization Of Chlorinated Solvents	17
The Markets For Chlorinated Solvents	19
IV. EMPIRICAL ANALYSIS	29
Overview of the Empirical Analysis	29
Model Specification: Systematic Effects	31
Model Specification: Error Structure	36
The Chlorinated Solvents Data Base	39
Estimation Results	43
Implications for Regulatory Policy	65
V. CONCLUSION	69
APPENDIX A: CHEMICAL STRUCTURE AND PRODUCTION TECHNOLOGY	71
APPENDIX B: QUALITATIVE HISTORY	76
APPENDIX C: ANALYSIS OF MARGINAL FEEDSTOCK COSTS	85
APPENDIX D: SPECIFICATION OF THE ERROR STRUCTURE	95
APPENDIX E: SAMPLE SAS PROGRAM APPROXIMATE GLS - SEEMINGLY UNRELATED REGRESSION WITH AR(1) CORRECTION	99
APPENDIX F: THE FUNCTIONAL FORM OF A PROXY FOR REGULATORY PRESSURE	107
REFERENCES	120

FIGURES

1. Chlorinated Solvents Production	22
2. Qualitative Events Time Chart	27
3. TCE: Predictions of a Single Equation Market Model	46
4. TCE Market Model: Predution versus Actual	49
5. PERC Market Model: Prediction versus Actual	50
6. TCA Market Model: Prediction versus Actual	51
7. METH Market Model: Prediction versus Actual	52
8. Simulation of regulation as a cost	68
F.1. Dynamic Proxies for Regulatory Pressure	109
F.2. The Logistic Function	110
F.3. Logistic Functions: Constant Inflection Point, Growth rate Varies	114
F.4. TCE Market Model with Trend Proxy: Prediction versus Actual	116
F.5. TCE Market Model with Logistic Proxy: Prediction versus Actual	117

TABLES

1. Numbers and Capacity Shares of Manufacturers of Chlorinated Solvents	19
2. Annual Production of Chlorinated Solvents	21
3. Share of Chlorinated Solvents in End Uses	24
3. Hausman Test, TCA Use Single Equation for Hausman Test for Endogenous Prices	35
4. The Specification of the Model for Chlorinated Solvents	43
5. Market Model Estimates, 1965-1975 Approximate GLS - Seemingly Unrelated Regression with AR(1) Correction	47
6A. Complete Model Estimates, 1965-1983 Approximate GLS - Seemingly Unrelated Regression with AR(1) Correction	55
6B. Complete Model Estimates, 1965-1983 Approximate GLS - Seemingly Unrelated Regression with AR(1) Correction	56
7. Price Elasticity Estimates	61
8. Complete Model on Constructed End Use Share Quantities OLS Single Equation Estimates	63
9. Price Elasticity Estimates from Constructed End Use Models OLS Single Equation Estimates	64
B.1. Perchloroethylene (PERC)	78
B.2. Trichloroethylene (TCE)	80
B.3. Trichloroethane (TCA)	82
B.4. Methylene Chloride (METH)	83
B.5. General Events	84
C.1. Input-Output Coefficients	88
C.2. Share of Chemical Cost in Material Costs	90
C.3. Elasticity of Production Cost with respect to Feedstock Cost	91
C.4. Marginal Feedstock Cost Series Equations for Generating estimates for Marginal Feedstock Costs	93
C.5. Marginal Feedstock Cost Series Estimates for Process Share of Total Production	94
F.1. Comparison of Linear Trend Proxies Market Model: 1965-1975	113
F.2. Comparison of Linear and Nonlinear Time Proxies Market Model: 1965-1975	115
F.3. TCE Complete Model: Logistic Proxy with Estimated Rate Entire Time Period: 1965-1983	118

THE MARKET RESPONSES TO THE GOVERNMENT REGULATION
OF CHLORINATED SOLVENTS: A POLICY ANALYSIS

Thomas W. Chesnutt

I. INTRODUCTION

The U.S. Environmental Protection Agency (EPA) receives notification of over a thousand newly created chemicals each year. The Toxic Substances Control Act (TSCA) charges the administrator of EPA with oversight of these chemicals in addition to all existing chemicals (GAO, 1984b). Needless to say, this is a monumental responsibility covering more than sixty thousand chemicals that have been used commercially (GAO, 1984a).

This research seeks to examine, qualitatively and quantitatively, the response of chemical markets to government regulation of toxic substances. In the past, the regulatory analysis guiding the implementation of TSCA has not fully accounted for the ability of chemical markets to substitute among similar chemicals. In order to understand the effect of government regulation, regulatory analysis needs a method to formally characterize dynamic role of market forces.

This study lays out one empirical methodology for use in regulatory analysis. The methodology presents a formal way to incorporate historical information on market behavior into the analysis of the effect of government regulation on related chemicals. This study demonstrates the methodology using one set of functionally related chemicals--the chlorinated solvents--and seeks to establish the scientific and institutional underpinnings of these related markets upon which to build a model that measures the market relationships. The approach taken looks back over the last twenty years of interactions in these chemical markets to measure the impact of previous government regulation.

Section II sets forth the policy context for this research. Section III provides analysis necessary to understand the chemicals involved, their production processes and costs, and an overview of their markets. Section IV specifies the systematic and nonsystematic portions of the formal model and then describes the Chlorinated Solvents Data Base (CSDB). Next, the empirical results generated by the estimation of

the model of markets for chlorinated solvents are presented. The validity of the chlorinated solvent model estimates are evaluated using other *a priori* information. Finally, possible applications of the model are discussed along with the implications for regulatory analysis.

II. BACKGROUND

THE TOXIC SUBSTANCES CONTROL ACT

Legislative History

The Toxic Substances Control Act (TSCA), passed by Congress in 1976, dates back to the National Environmental Policy Act (NEPA) that President Nixon signed into law on January 1, 1970 (P.L. 91-190). The NEPA created a national policy for the environment and established a new organization within the executive branch, the Council on Environmental Quality (CEQ), to make recommendations to the president on policy initiatives to improve environmental quality. After more than a year of evaluation the CEQ concluded that existing laws were inadequate to control the dangers posed by toxic substances. In a report titled Toxic Substances (CEQ, 1971), the CEQ concluded that the problem of toxic substances required a comprehensive and systematic approach and recommended a Toxic Substances Control Act as the best means to bring this about. The Act would require testing of new chemical compounds, collect information about chemical production and uses, and control chemicals harmful to human health or the environment (CEQ, 1971, pp. 21-22).

The original draft of the TSCA bill--written by the CEQ and introduced with administration backing as H.R. 5276 in the House and S. 1478 in the Senate--fell victim to a heavy lobbying effort by the chemical industry (Dolgin, 1974, pp. 155-157). Spearheaded by the American Chemical Association, Dow Chemical, Du Pont, and the Manufacturing Chemists Association (now the Chemical Manufacturers Association), the lobbying by chemical interests succeeded in preventing passage of the bill for about five years. It took the occurrence of two toxic substances incidents in 1975 to bring about TSCA's passage.

During the 94th Congress, legislation to enact TSCA was introduced in the Senate as S. 776 and in the House under several different versions. Though the Congress had received testimony in the previous four years of debate on mercury poisoning, the carcinogenicity of diethylstilbestrol, the effect of PCBs, and other potentially harmful

chemical compounds, two separate incidents came to light in 1975 that seemed to activate public concern over toxic substances. In January came confirmation of link between worker exposure to vinyl chloride and angiosarcoma of the liver, a form of cancer (Doniger, 1979). Then in June it became known that workers in a small Virginia manufacturing plant had sustained severe neurological and reproductive damage from contact with the chemical Kepone. These two events brought heavy public criticism of the federal government for its failure to foresee and prevent these tragedies and gave the needed impetus for the final passage of the TSCA on September 28th. President Ford signed the bill into law on October 11, 1976 as Public Law 94-469 (Druley and Ordway, 1977).

Implementation

Originally conceived as fill-gap legislation, the TSCA tasks the administrator of the Environmental Protection Agency (EPA) with oversight of all chemicals having the potential for toxic effects¹. In particular, the general policy statement of the Act lists three objectives:

- to develop adequate data on the health and environmental effects of these chemicals,
- to regulate chemicals which present an unreasonable risk to health or of environmental injury, and
- to avoid undue impediments to technological innovation.

The Act gives the EPA Administrator broad discretionary powers to pursue these goals. Within the EPA, the implementation of this mandate has been delegated to the Office of Toxic Substances (OTS). The TSCA distinguishes between the regulation of "new" chemicals and that of "existing" chemicals. A short description of regulatory activity in both areas is followed by a discussion of their shortcomings.

¹It exempts pesticides and certain other classes of chemicals that are regulated under other statutes.

New Chemicals: The OTS must review over one thousand new chemicals each year for possible toxic effects. Based upon the information provided in a Pre-Manufacturing Notice (PMN), the OTS must decide what, if any, regulatory action is necessary. A few chemicals considered most dangerous have, since the passage of TSCA, been required to undergo animal testing to determine the nature and extent of the threat. Without negative test results the EPA will not allow the chemicals on the market. Firms frequently withdraw the PMN, preferring to avoid the high cost of testing.

Since the premanufacture requirement became effective in July 1979, the EPA has received over 4000 PMN's. The great proportion of these, approximately 95 percent, have been approved (GAO, 1984b). One may infer from regulatory practice that the EPA has stringently interpreted what constitutes "unreasonable" risk from chemical substances. The EPA feels it must have substantial evidence of hazard in order to require testing of a chemical. Though this may appear as a reasonable working hypothesis, the analytic methods used to assay the hazard rarely produce conclusive evidence².

The fundamental tension between the regulatory need to make decisions today and the scientific leaning to avoid judgment until the conclusion is certain, found expression on both sides of the political controversies over the regulation of toxic substances. Environmental groups attributed the languid implementation of TSCA to "paralysis by analysis," suggesting that the "cost-benefit analysis" called for in Reagan's Executive Order 12291 was only a political lighting-rod for avoiding the promulgation of any new regulation based on TSCA (North, 1983). Industry, on the other hand, dispaired at the absence of explicit rules on the nature of information required in PMNs, what reporting was needed, and the amount of new record-keeping mandated by EPA rules (*Wall Street Journal*, 9 July 1980).

² For a good overview of the controversy surrounding testing methods, see the article by Arlen J. Large in the *Wall Street Journal*, 21 June 1983.

The political turmoil surrounding the implementation of the new chemicals section of the TSCA naturally spilled over into the courts. The caution shown by the EPA in its implementation of TSCA has been attributed by many to the intrusion of the judicial system into regulatory rule-making. When the EPA promulgated rules under Section 5c, it solicited comments from the public. It received over 200 comments contained in no less than 4000 pages; no legal or analytic justification escaped criticism³. Personnel within the EPA worried that in-house legal review was preventing timely implementation.⁴ This is not to imply that the in-depth legal analyses avoided legal action over EPA rules. To the contrary, *Science* magazine pointed out that in 1979 the EPA was facing over seventy lawsuits (*Science*, 1979) concerning their rule-making. Although the stakes involved under each case may have been limited to one company or one chemical, the implications in terms of precedence loom much larger. In any case, the confluence of agency rule writing and judicial rewriting have lead many to question where the authority for the implementation of TSCA ultimately lies. As one pundit put it, "Where the New Dealers had hoped to replace the inefficient courts with efficient agencies, we now have inefficient agencies and inefficient courts. (Robert Kaus in *Washington Monthly*, July-August 1979).

Judicial decisions have powerfully influenced the EPA's implementation of the new chemicals section of the TSCA. An early civil suit filed by the Natural Resources Defense Council in 1980 pointed out that the EPA had missed every legislated deadline for making testing decisions on chemicals (*NRDC vs. Costle*, 1980). The EPA in an out of court settlement agreed to clear the backlog of chemicals and to meet a one year deadline for making the decision on whether to test a chemical. To meet the deadlines, the EPA relied on "negotiated test agreements,"

³See the affidavit of Steven Jellinek (1979, p. 24) for more detail.

⁴"There was a sense here before that the lawyers had to have the last *i* dotted and *t* crossed before we could go anywhere," said John Todhunter, assistant administrator for pesticides and toxic substances (*Fortune*, 20 Sept. 1982).

voluntary settlements with commercial manufactures of chemicals recommended for testing (Worobec, 1984). The NRDC and the AFL-CIO challenged the voluntary program in another suit; the Federal District Court ruled that negotiated agreements did not meet TSCA requirements⁵. EPA then submitted a rule-making schedule to the Court (N.Y. Times, 30 Sept. 1984). The controversies over the regulation of new chemicals are likely to continue in the judicial system, adding further uncertainty to the regulatory task facing the EPA.

Existing Chemicals: Currently, over 65,000 chemicals are used in commerce and, of these, only a few thousand have been tested for chronic toxicity. Many of these tests were performed years ago under testing protocols considered inadequate today⁶. Thus only a small fraction of chemicals tested have valid testing results. Further, the EPA has no programmatic method for testing across various types of chemicals. One finds the greatest amount of testing in a few chemical types and almost none in others.

The EPA has invoked the provisions of the TSCA in only four cases. The first was the ban on chlorofluoro chemicals used as aerosol propellants. The second case involved the requirement for inspection of schools for asbestos. The third and fourth concerned dioxin and PCBs. These actions have been characterized as reactive: a bureaucratic response to a politically explosive situation. A regulatory policy reacting mainly to political fires leads to two types of failures: 1) regulating too much too late, and 2) creating perverse incentives for discovering future problems.

⁵ Judge Kevin Duffy used a particularly harsh tone in his judgment, asserting that the EPA's enforcement of the TSCA "subverts the statutory scheme" and its explanations of its policy were "specious" (L.A. Times, 14 Sept. 1984).

⁶ The National Research Council found only 27 percent of 664 toxicity tests examined met the most basic requirements of protocol design, conduct of research, or reporting of results (*Research & Development*, 1984).

Problems with the Implementation of TSCA

Critics believe the original intent of the TSCA has been largely thwarted in the first ten years of its implementation. The Government Accounting Office conducted a review in 1980 that concluded: "neither the public nor the environment are much better protected." Since then, environmental groups have grown more vocal, accusing the EPA of ignoring legislative mandates of TSCA in order to accommodate chemical manufacturers. Congressional dissatisfaction with current policy resulted in two GAO investigations, both highly critical of EPA policy. Representative James J. Florio (Democrat, New Jersey), in reaction to the GAO reports, summarized the critical view of the EPA's implementation of TSCA: "...the EPA does not effectively screen new chemicals, has failed to issue major regulations controlling existing chemicals, and has not established a credible enforcement program" (N.Y. Times, 10 July 1984).

The difficulty of implementing the TSCA has been traced to constraints beyond the control of the EPA--complexity and ambiguity of the original legislation, lack of resources to adequately follow through on the legislated mandate, and in the last seven years, lack of political support for new regulation (Woodhouse, 1985). This research, however, will be directed toward how regulatory analysis can make for better regulatory decisions *within* these constraints.

The Role of Regulatory Analysis

For analytic purposes the shortcomings of TSCA will be looked at along lines suggested by the distinction made between "new" and "existing" chemicals in the legislation. Each year, manufacturers submit PMN's for about 1000 new chemicals. Since the decision maker faces the same decision making context each year, the analysis of this context will be termed a *static* view. In contrast, chemicals in current use have an interesting history with respect to both market forces and government regulation. The analysis of the history of existing chemicals will be termed a *dynamic* view.

A Static View: The implementation of the TSCA can be viewed in the static sense of inadequately coping with an information sparse world. In the 1984 report, the GAO singled out the new chemical review program as an area of "major weakness" (GAO, 1984b). Though the GAO related some of the problems to a lack of funding, other problems were traced to the information content of the PMN's. One year earlier, an Office of Technology Assessment analysis revealed that only 53% of the PMN's examined contained any toxicity data (OTA, 1983). Of these, the toxicity data provided were rarely of the kind to provide good indication of the potential negative effects on human health. The GAO further pointed out that the EPA had performed only 11 investigations to find out if chemical manufactures were providing notice or supplying reliable information in the PMN's.

Instead, the EPA has been forced to rely on a type of analysis known as Structure-Activity Relationship (SAR). The validity of this approach has been attacked on two levels. First, some question the premise of SAR analysis that chemicals having similar molecular structures will also share a similar toxic threat. Second, the method critically depends on how much is known about the toxicity of existing classes of chemicals. Even if a new chemical can be matched to an existing set of chemicals, little can be inferred about the new chemical if little is known about the existing chemicals. In 1984, a National Research Council panel examined the 675 chemicals for toxicological information and found only 20 percent of the test performed on commercial chemicals contained even minimal information and found virtually no information about the hazards of exposure to the other 80 percent of the chemicals (*Research & Development*, 1984). Critics suggest that the narrowness of the present state of knowledge about the toxic effects of chemical substances precludes useful inference based upon SAR analysis.

Though Congress intended the TSCA to increase the amount of testing for chemical toxicity--as explicitly stated in Section 8 of the Act--most chemicals identified by the EPA as potentially dangerous are not tested. This is due to the fact that the manufacturing firms must themselves pay for the expensive animal testing. Rather than pay for the

sure expense of animal tests for proof of an uncertain level of toxicity, most firms will simply retract the PMN and never produce the chemical. Unless the EPA can extract a voluntary testing agreement, it cannot validate the initial judgment as to the toxicity of the chemical. Given the uncertainties inherent in the available analytic procedures, this lack of feedback can withhold the information needed to validate and improve the analysis.

A Dynamic View: Another problem area relates to the dynamics of competition among chemicals already on the market. The regulatory analysis supporting the implementation of the TSCA has, in the past, overlooked the market response to government regulation. Markets respond not only by *anticipating* government action, but by quickly substituting to other less regulated chemicals, before and after government regulation. Again in an information sparse world, it is entirely conceivable that the government would induce firms to switch from chemicals about which the government knows more, to ones about which it knows less. These chemicals could have the same inherent level of toxicity; only the knowledge of toxicity varies. Firms could be forced to bear the costs of substituting among chemicals, with no reduction in absolute level of risk faced by society. Indeed, with the previous focus on regulating chemicals one at a time, firms could be forced to switch several times among chemicals, dependent upon which chemicals were under government scrutiny. The dynamic response of chemical markets to government regulation--the ability of markets to substitute in ways not foreseen by the government--lies at the crux of my proposed analysis.⁷

⁷The analysis of the dynamic response of markets to government regulation forms the analytic focus for this research. This is not to suggest there are no productive analytic venues for addressing the static problem--an unknown threat posed by the thousand new chemicals reaching the market every year. Theoretically, the situation could be analyzed within the framework of game theory as a game played repeatedly through time. Practically, since very little data exist to evaluate present or future government practices, simulation methods could be used to highlight the implications about different possible states of the world.

The Case of Chlorinated Solvents

The markets for one set of functionally related chemicals--chlorinated solvents--form the subject of this analysis. Constraints on analytic resources prevent such an intensive effort for all chemical markets, but a research focus on a narrow subset of markets offers both theoretical and practical advantages. A focussed approach allows us to empirically control for confounding factors. I then isolate the relevant relations that illustrate the inherent risk dynamics of market substitution. The chlorinated solvents are also a interesting practical subject because all of them pose health or environmental threats: there is known substitutability among them, a history of active government regulation, and current regulatory interest.

Uses of chlorinated solvents occur throughout the economy and defy simple technical categorization. They range from degreasing metal parts for office furniture to the dry cleaning of clothes. Using publicly available data on the production and market price of chlorinated solvents, regulatory action, and economic forces, this analysis applies formal methods to handle market linkages. The next section will discuss alternative approaches to the analysis of toxic substances before we present our approach.

ALTERNATIVE APPROACHES

Risk Assessments

One type of analytic approach important to regulatory decision making takes the form of a risk assessment. This is a formalized aid to decision making under risk: "a heterogeneous conglomerate of theoretical and methodological approaches from various disciplines" (Conrad, 1980, p. 248). Risk assessment as a form of study has been around since the formation of insurance companies in fourteenth century Spain for the purpose of sharing the risks of maritime shipping. Two fairly recent historical developments have spurred the growth and methodological form of risk assessments.

Much of the newly emerging field of risk assessment gained its impetus from a little noted section of the National Environmental Policy Act (NEPA) of 1969 that required an environmental impact statement on all federal projects--an empirical assessment of the possible impacts (outcomes) and their relative likelihood. The environmental impact statement soon turned into a major piece of analysis crucial to the success and public acceptance of any project. Within a few years, a large body of professionals had formed to fulfill just this function (Kates, 1977).

The methodological development of risk assessment was shaped by the battle of the nuclear power industry to establish, in their own environmental impact statements, that the benefits from electricity generated by nuclear plants outweighed the risks. Due to limited experience with nuclear power, very little hard evidence was available upon which to base empirical risk assessment. The nuclear industry responded with the creation of several hypothetical risk models whose influences remain in the methodology of present day risk assessments. To generate an empirical measure of risk, these models needed to make intuitively difficult but computationally simplifying assumptions.

Criticisms of Risk Assessments

The growing professionalism in risk assessment brought about by the environmental impact assessment requirement of the NEPA and the theoretic bent of many of the empirical risk estimates far from settled all questions over acceptable risks to society. In fact, the attempt to convince the public of the validity of technical estimates of risk often served more to erode trust in technical expertise than to assuage public concern over a new undertaking. Many studies were attacked more for what remained unanalyzed than for the methodology of what was analyzed. Poorly defined or measured issues that could be handled approximately are shirked in order to preserve rigorous treatment of narrowly defined problems.

Risk assessments are often criticized for construing risk solely in terms of human mortality, instead of taking a broader view defined by Rowe (1977) to include:

risks to health and life, such as those resulting in pain, disability, or premature death; risks to the environment, either local or global and having reversible and irreversible effects; risks to the economic well-being of groups; and risks of changes in the status quo of certain individuals or groups.

In this vein, a risk assessment for chlorinated solvents would gather all the relevant technical knowledge about the chemical posing a risk, identify the nature and characteristics of the risk, portray the important economic relations, and provide an institutional context. Moreover, a risk assessment must also incorporate how people perceive the risk and what, if anything, should be done to lessen the risk. Due to the need for inclusiveness, many risk assessments end up as a very large document, the worst giving the appearance of an encyclopedia. Needless to say, lack of accessibility through volume alone will hinder social consensus on an acceptable level of risk.

Risk assessments tend to focus on a single point in time, taking a static view of everything known about the risk. This is a specific version of a more general forest and trees problem. Demonstration of mastery of technical minutiae does more to fend off critics, or at least bore them into silence and is surely much safer than a strong assertion of actions needed in the immediate future.

Though risk assessments handle the probabilistic parameters sufficiently well they often inadequately acknowledge the extent of uncertainty--the ignorance about the parameters and how they change through time. Much of the risk research avoids explicit consideration of how uncertainty changes the empirical results of risk models. In general, much of the interesting texture and detail that drive technical and economic change through time end up in the analytic waste bin.

Linear Programming Model

A more formal method for dealing with a change through time has been proposed in the form of a linear programming model. Danzig developed a methodology, or program, to find solutions to systems of linear equations. The problem is constructed with a linear function that specifies what is to be valued, the objective function. One tries to minimize (or maximize) what is valued, given a set of constraints representing the limitations due to the laws of nature, economics, or people.

A useful application of a linear programming model to examine changes in the related markets for chlorinated solvents will specify the costs of production and use of solvents as the objective function. A set of constraints would include the requirement that 1) production of end products meet or exceed the final demand for that end product, 2) solvent supply equal solvent demand, and 3) a solvent plant not produce more than its capacity. Regulations on the solvents could also be included as separate constraints governing their use. Such a model could play out the comparative static exercise of predicting the change in the total cost of use and production of a solvent brought about by a change in regulatory constraints or technology. Prices, in the above model, are an endogenous artifact. They show the after-fact shadow worth of a solvent, in production and consumption, after the one step move to equilibrium.

The voracious data demands of a linear programming model form one of the major limitations to translating a move away from present reality. In order to successfully predict the shifts in demand brought about by regulation, one must have very accurate information on the particular production technologies and user's ability to substitute alternative solvents. In this sense, a linear programming model can only show the effects of known technical options; hence it specifies not so much a market reaction but a technical reaction.

MARKET RESPONSE: THE APPROACH

Given that risk assessments tend to make simplifying assumptions about behavioral relations in economic markets, how can one attempt to better capture the response of economic markets to government regulation? This analysis takes a historical approach, looking back to a practical and interesting case where chemical markets responded to external pressure. The chlorinated solvents form the subset of functionally related markets in this analysis.

The historical analysis follows two tracks: a technical analysis to identify the important scientific and institutional relationships and a empirical analysis to measure and formally link up these relationships. Both tracks require a solid understanding of much technical detail: the chemical structure and properties of the solvents, the technology used to produce the solvents, the technical process requiring solvents as an input, and the regulatory history surrounding these chemicals. Sound technical knowledge not only forms the basis for the technical analysis, but takes an equally important role in creating and validating a usable formal model of the markets for chlorinated solvents. For this reason, the technical analysis naturally precedes the empirical analysis.

III. TECHNICAL ANALYSIS

This section provides the technical analysis necessary to understand the interaction of production and use of chlorinated solvents. The construction of a model of chlorinated solvents that usefully enumerates this interaction necessitates a solid understanding of these technical underpinnings.

First, the chlorinated solvents are introduced with a brief synopsis of their origin and commercialization. Next, the economic markets for chlorinated solvents are addressed with an overview of their structure, the historical production levels, the various end uses, and regulatory actions taken against the chlorinated solvents.

HISTORY OF THE ORIGIN AND COMMERCIALIZATION OF CHLORINATED SOLVENTS

Chlorinated hydrocarbons have been in existence since 1821, when Faraday formed perchloroethylene by the thermal decomposition of hexachloroethane.¹ Development of other chlorocarbons continued throughout the early part of that century. Liebig derived chloroform in 1831 by treating chloral with an alkali. Dumas and Peligot produced a form of methyl chloride by heating methanol with sulfuric acid and sodium chloride in 1835. By 1839 Regnault had obtained carbon tetrachloride by chlorinating chloroform. Then in 1840 he chlorinated methyl chloride in sunlight to produce methylene chloride and was later able to isolate 1,1,1-trichloroethane. Fischer formed trichloroethylene by reducing hexachloroethane with hydrogen in 1864.

Although chloroform was the first to develop large commercial applications, as one of the early general anesthetics, it was later displaced by other more effective and less toxic compounds. Large scale commercialization of other chlorinated solvents did not occur until the early 1900s when a process for liquifying chlorine became commercially viable. This transportable form of the raw material chlorine opened

¹Material for this section and the next come primarily from Merck (1985), Kirk-Othmer (1985), and Considine (1984).

commercial possibilities for chlorinated solvents. The growth of markets for chlorinated solvents have been strong ever since, rivaling the rapid expansion of petrochemical markets.

Chloroform, carbon tetrachloride, and methyl chloride have now been supplanted in most of their original end uses. Presently they are primarily used as intermediates in the production of other chemicals. Several other chlorinated solvents, however, find commercial application in the wide variety of end uses that accounted for the rapid market growth for chlorinated hydrocarbons. These solvents compete vigorously for position in rapidly changing markets. Though many of the chlorinated solvents can substitute for others, each possesses individual chemical characteristics that render it more or less suited for a particular application. The overlap of economic and technical suitability has made for a complex history of interaction among the chlorinated solvents in the last twenty years.

For the purposes of this study, only the most commercially important chlorinated solvents were selected for analysis. The following are the names and abbreviations for these chlorinated solvents:

<u>Chemical</u>	<u>Abbreviation</u>
Chlorofluorocarbon 113 (Trichlorotrifluoroethane)	CFC-113
Methylene chloride (Dichloromethane)	METH
Methylchloroform (1,1,1,-Trichloroethane)	TCA
Perchloroethylene (Tetrachloroethylene)	PERC
Trichloroethylene	TCE

The chemical structure for these chemicals may be found in Appendix A.

THE MARKETS FOR CHLORINATED SOLVENTS

This section presents an overview of the markets for the five major chlorinated solvents, beginning with a discussion of their economic structure and then moving to a description of their historical production levels, end uses, and regulatory history.

Economic Structure of the Markets

These markets can be characterized as oligopolistic with few producers and, until recently, very limited foreign competition. Table 1 shows the number of domestic firms in 1986 and the relative share of total capacity of the top two firms.

Though the actual market shares of each producer would be more informative, these data are not published. Even the total level of production of a chemical will not be reported by the Bureau of Commerce if the number of producers is less than three. (One producer would then be able to infer the exact level of production of the competitor.) This data constraint only comes into play for two chemicals. Total production data for TCE is unavailable after 1983, when the Ethyl plant in Baton Rouge shut down. Accurate historical production data for CFC-113 is completely unavailable as only two firms have produced it. Intelligent estimates can be made as to the annual level of CFC-113 production, but the lack of hard data will preclude its use in a formal empirical model.

Table 1

NUMBERS AND CAPACITY SHARES OF MANUFACTURERS OF CHLORINATED SOLVENTS

	Number of Manufacturers	Share of Total Capacity, Largest Two Manufacturers
TCE	2	100
PERC	5	46
TCA	3	80
METH	5	71
CFC-113	2	100

Note: Data taken from the *Chemical Marketing Reporter* profiles.
The data for METH reflect 1983 information.

production, but the lack of hard data will preclude its use in a formal empirical model.

Features about the production processes can greatly complicate the economics of chemical markets at the level of the firm. (Appendix A documents the production technologies for each chemical.) Many of the chemicals are jointly produced with other chemicals or are used as feedstocks in the production of derivative chemicals. When sold, the chemicals often go through one or more distributors who repackage or combine the chemicals with other chemicals or with one another for specific end uses. In sum, the complexities of all the market linkages and relationships cannot be contained in any one analytic model. Instead, this study shall focus on the final derived demand for the chlorinated solvents.²

Historical and Present Solvent Production

Table 2 shows annual production for each chlorinated solvent from 1964 through 1985. Figure 1 graphically displays quarterly production, smoothed by an annual moving average. The data for PERC, TCE, TCA, and METH were taken from the International Trade Commission Reports (ITC).³ Because CFC-113 is manufactured by only two producers, production data are not reported to the International Trade Commission. The values in Table 1 were estimated using the published literature and input from producers.

An intermediate goal of the empirical analysis will be to understand the determination of the historical production levels. Toward that end, the movement of production levels over time will be briefly described for each of the chemicals.

²Wolf and Camm (1987) address other related issues such as the economic viability of recycled solvents and the economic costs of the disposal of their wastes.

³These reports were known as the U.S. Tariff Commission Reports before 1974.

Table 2

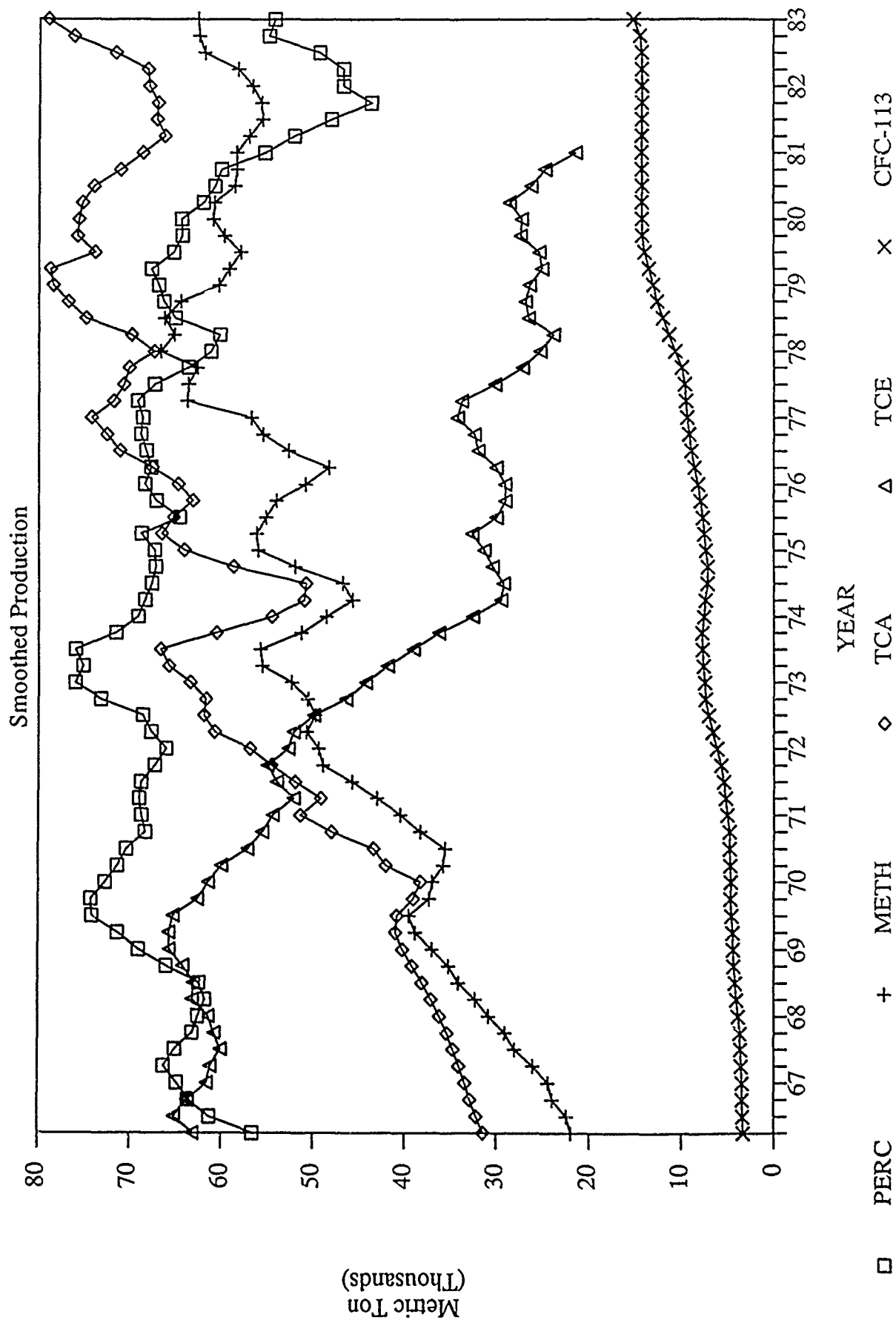
ANNUAL PRODUCTION OF CHLORINATED SOLVENTS

(In thousands of metric tons)

Year	TCE	PERC	TCA	METH	CFC-113
1964	168	166	-	-	12
1965	197	195	-	-	12
1966	218	210	110	-	13
1967	222	242	126	119	14
1968	235	289	136	137	15
1969	271	288	147	166	17
1970	277	321	166	182	19
1971	234	320	170	182	19
1972	194	333	200	214	22
1973	205	320	249	236	29
1974	176	333	268	276	31
1975	133	308	208	225	29
1976	143	303	286	244	31
1977	135	279	288	217	37
1978	136	329	292	259	39
1979	145	351	325	287	50
1980	121	347	314	256	57
1981	117	313	279	269	57
1982	103	265	270	241	57
1983	276	248	266	265	57
1984	-	260	306	275	68
1985	-	224	268	263	73

SOURCE: U.S. Tariff Commission Reports (1964-1973) for TCE, PERC, TCA, and METH; U.S. International Trade Commission Reports (1974-1985) for TCE, PERC, TCA, and METH; RAND estimates for CFC-113.

Fig. 1: Chlorinated Solvents Production



TCE production grew steadily through 1970 and declined steadily thereafter. The events that led to this decline are detailed below. In later years--1984 and 1985--production data for TCE were not published by the ITC since all but two producers had closed their plants by then.⁴

The PERC production data show continued growth through the mid-1970s, a slight dip, and strong growth again through 1981. The significant decline in recent years is a result of several factors mentioned in the regulatory history section but discussed in much more depth in Wolf and Myers (1987).

TCA production levels increased over the twenty year period, with a decline in 1982 and 1983 because of the recession. Production of TCA is presently higher than for all other solvents, illustrating its technical diversity.

METH production exhibited strong growth in the early years and sustaining levels from the mid-1970s onward. The solvent is currently under regulatory scrutiny by EPA's Office of Toxic Substances.

CFC-113 production is lower than that of any other solvent in Table 2. Nevertheless, its growth in the last decade has been startling and has been much greater than that of the other solvents.

Production of at least four of the five solvents declined in 1985. Because of the strong dollar in that year, imports increased and exports decreased significantly. It is notable that the lower production levels reflect this trend and that demand for the solvents in the United States did not necessarily decline. Any empirical analysis must make the distinction between the domestic production of Table 2 and domestic use. Thus the empirical analysis of the next section will arrive at a better proxy for total U.S. use by subtracting out exports and adding in imports to production values.

⁴The large jump in reported TCE production in 1983 may reflect stockpiling by the manufacturer that stopped producing in 1984.

Solvent End Uses

Each solvent is used in a variety of diverse applications. Table 3 provides a brief summary of the linkages between end uses and solvents; it shows the share of the production of a chlorinated solvent taken up by a particular end use in one year. These estimates come from Wolf and Camm (1987), which may be referred to for a more thorough analysis of end uses. For the present purposes, the outline of uses in Table 3 will serve as the preliminaries to understanding the basis for the model of chlorinated solvents and to give a flavor of the range of solvent applications.

Most of TCE is used in metal cleaning, although some is used as an intermediate in a polymerization reaction of vinyl chloride. Miscellaneous uses include fabric scouring, adhesives, fungicides, paints and pharmaceuticals.

Table 3
SHARE OF CHLORINATED SOLVENTS IN END USES

	TCE	PERC	TCA	METH	CFC-113
Metal Cleaning	80	10	63	8	15
Dry Cleaning & Textile Processing	-	53	-	-	3
Adhesives	-	-	10	-	-
Aerosols & Foam Blowing	-	-	7	25	-
Electronics			6	7	52
Paint Remover	-	-	-	23	-
Chemical Processing & Intermediate	5	28	4	20	-
Miscellaneous Uses	15	9	10	17	16

SOURCE: The *Chemical Marketing Reporter*.

More than half of PERC production ends up in dry cleaning and textile processing applications. The production of CFC-113 uses a significant portion of PERC as a chemical intermediate. Some PERC is used in metal cleaning, and miscellaneous uses include grain fumigation, automotive cleaners, household products, and pharmaceuticals.

The majority of TCA production goes toward metal cleaning end uses, although it also finds application in a wide range of other uses: adhesives, aerosols, electronics, and as a chemical intermediate for vinylidene chloride. Miscellaneous uses include textile scouring, drain and septic tank cleaners, grease cutters, pharmaceuticals, and the weatherproofing of leather products.

Paint removers, aerosols, and chemical processing form the major uses of METH. METH also finds significant application in the cleaning of electronics and metal parts. Other uses include decaffeination of coffee and spices, grain fumigation, and mildew proofing.

About half of CFC-113 production is used in the electronics industry for critical cleaning and the defluxing of printed circuit boards. It is also used in metal cleaning and, to a lesser extent, for the dry cleaning of specialty items. Miscellaneous uses include the manufacture of polyolefin foams, refrigerants, and a fluoropolymer. It is also used as a cutting fluid and as a reaction and carrier medium.

Regulatory History: Qualitative Timeline

During the last two decades, several events have influenced the metal cleaning use of chemical solvents. Such events include regulation or proposed regulation of various types and various changes in market conditions. Markets do not straightforwardly react to such exogenous shocks--some events are expected and others surprise. Because this nonstandardized response to unknown forces prevents easy numerical representation, knowledge of these events is retained in a qualitative form. Awareness of the larger forces acting on chemical solvents and metal cleaning markets must be melded into any quantitative analysis of these markets.

Take, as an example of a regulatory event, a change in the regulated Threshold Limit Value (TLV). The Threshold Limit Value is the maximum allowable time-weighted average concentration to which a worker may be exposed over an eight-hour working day, five-day work week. Generally, chemicals of higher toxicity will have a lower allowable TLV. Lower TLVs, in turn, imply that higher costs will be incurred in the production process. This is due to the additional expense of the control technologies needed to comply with the more stringent TLV standard. The exact nature of the market response to a change in the mandated TLV will depend on the particular chemical, the availability of substitutes, and the degree to which this regulatory event was anticipated.

Figure 2 summarizes these events for each chemical solvent in the form of a timeline.⁵ Appendix B contains a more complete description for each chemical and includes some general events that may have influenced the use of all of the solvents.

PERC: Most of the changes in the TLV for PERC occurred before the relevant period of study. It's level of production has been closely linked to the production of chlorofluorocarbons which use PERC as a feedstock. The use of PERC as a solvent increased through the early 1970's as users substituted away from other solvents but negative test results showing adverse effects slowed this gain in the late 1970's.

TCE: A powerful and relatively cheap solvent, TCE found wide application in metal cleaning end uses during the 1960's. Its use began to slacken when local governments began to regulate it as a possible photoreactive substance. Los Angeles County became the first and most notable case in 1969 with others following suit in the ensuing years. Positive carcinogenicity test results in mice and EPA restrictions on emissions hastened the decline of TCE use in the 1970's. The ACGIH recommended its TLV be further lowered in the early 1980's⁶ and use can be expected to decline in the future.

⁵I exclude CFC-113 because it still retains the highest TLV permissible and a recent animal test was negative. In effect, it has experienced no binding regulatory events although it is presently under EPA scrutiny as a suspected ozone depleter.

⁶Though the Occupational Safety and Health Administration (OSHA)

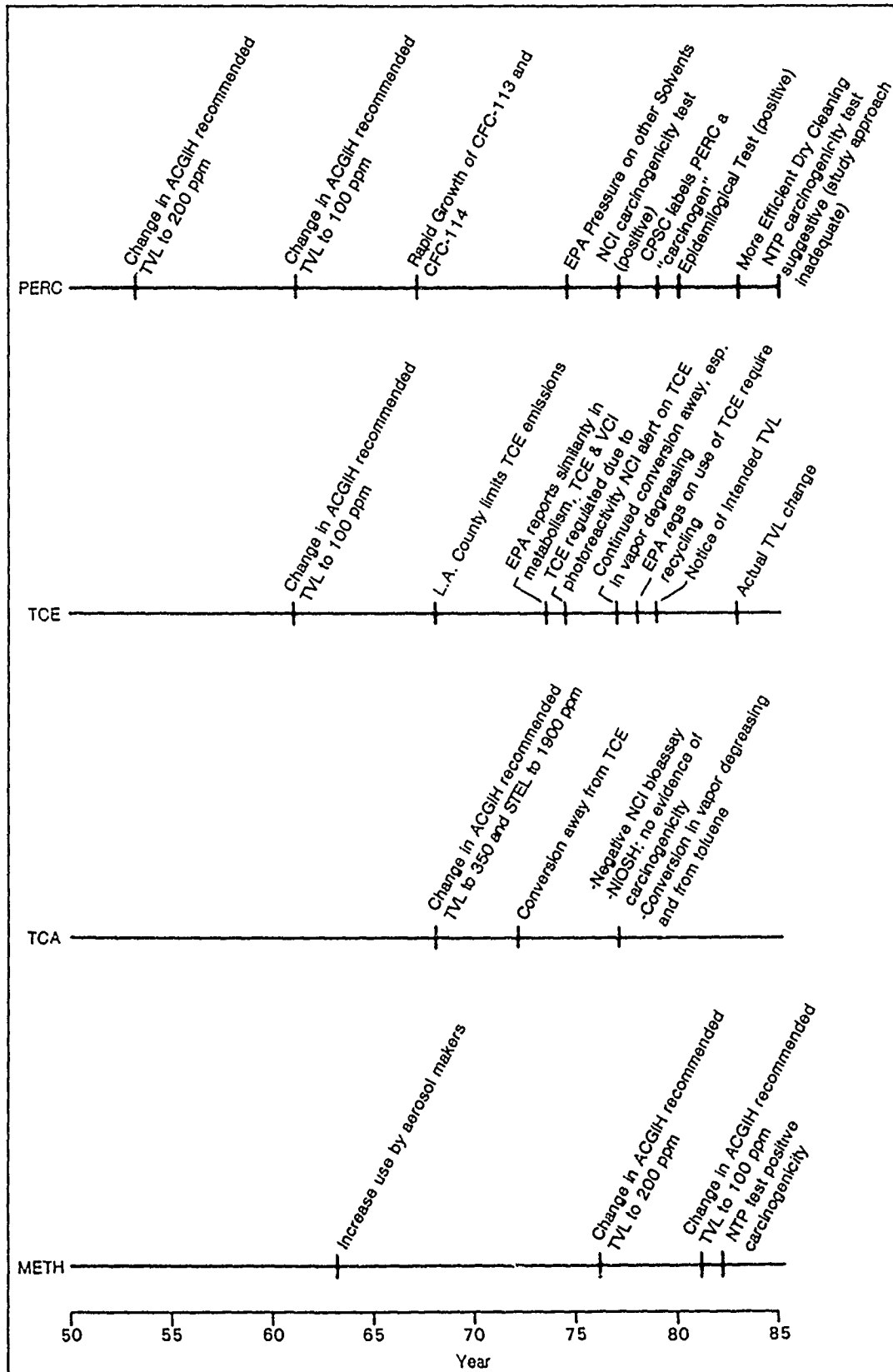


Fig. 2 — Qualitative events time chart

TCA: TCA has become the solvent of choice in a host of diverse applications. Though the ACGIH recommended its TLV be lowered in 1968, it came to be the substitute solvent that captured much of the TCE market. Most test results have proved inconclusive.

METH: Methylene chloride is a popular degreasing agent that has more recently come under scrutiny as a possible carcinogen. The ACGIH recommended its TLV be lowered in 1976 and the recommended level was cut in half again in 1981. Test evidence of carcinogenicity may limit its future growth.

sets the legal TLV limit, the American Conference of Government and Industrial Hygienists (ACGIH) recommends TLV levels that are often more conservative and are widely adhered to by responsible manufacturers and users.

IV. EMPIRICAL ANALYSIS

OVERVIEW OF THE EMPIRICAL ANALYSIS

Given the background provided by the technical analysis of the last section, we now turn to the construction of a formal econometric model to enumerate the the forces that drive the markets for chlorinated solvents. The discussion of this empirical analysis will be broken down into conceptually distinct subsections: the model specification, the data, the estimation results, and the evaluation of the model. This overview provides an introduction to the modeling concepts addressed in each subsection of the empirical analysis.

Model Specification

The econometric methodology employed to specify the model for chlorinated solvent use is broken into two distinct parts--systematic and nonsystematic effects. First, a model must specify how systematic forces can change the use of solvents. This "structural form" of a model defines how the these systematic effects occur. Next, a model must specify the nature of nonsystematic forces: how observations may randomly depart from the (hyper)plane defined by the structural form. Any information contained in the nonsystematic effects can be used to improve the estimates of the systematic effects. It should be noted, however, that specifying the systematic form of a model has much greater implications for estimation than the specification of the nonsystematic form. Misspecification of the structural form will lead to estimates of model parameters that are biased (off target) and even inconsistent (biased with increasing sample size). Specification of nonsystematic form--though improving efficiency (a nontrivial issue with the limited data available)--cannot correct for the bias of a misspecified structural form.

The specification of systematic forces in the model are laid out in a logical progression to show the derivation of the final model form. Emphasis is placed on the features of the structure that allow price

effects to be identified, since the direct effect of solvent prices, in turn, identifies the main workings of the solvent markets. A short discussion of the difficulties in measuring regulatory effects concludes the subsection describing the specification of systematic effects.

The specification of nonsystematic forces in the model follow under the title of "Error Structure." There will be randomness associated with the systematic model above, since every point will not lie on the regression plane. The nonsystematic error in the model is defined by the vertical distance of any point from the plane defined by the systematic model. If there are patterns associated with the random errors of a model, the information in this "structure" must also be specified to obtain, in our case, efficient estimation. The specification of the error structure entails setting forth what departures from pure randomness may be expected, tests for the different types of patterns, and a method for incorporating the information contained in the nonsystematic forces into the estimation of the systematic forces. The error structure is derived analytically and a method of estimation is set forth in a series of steps.

Data

The estimation of a formal model critically depends on the quality and availability of data describing the phenomenon to be modeled. Furthermore, the validity of the enumeration will also determine the validity of statistical inference from a formal model. Hence, it is natural to review of the empirical measures available for modeling before discussing the statistical estimation of the model.

The Chlorinated Solvents Data Base contains measures of aggregate solvent use, solvent price, and indices of the level of economic activity in the sectors of the economy that use solvents. This subsection presents the origin of these data and issues related to their validity.

Estimation Results

At the heart of the empirical analysis stands the measurement of regulation's effect on the markets for chlorinated solvents. The first step toward measuring regulatory effects involves the construction of a model that describes the linkages among the solvent markets without regulation. Only when a market model has been constructed, can regulatory forces be separated from market forces.

The last subsection documents the effect of regulatory pressure by comparing a model of solvent use that captures only market effects with the actual use of solvents under regulation. An evaluation of the behavior of the model then precedes a discussion of possible proxies for regulatory pressure. Finally, the model estimates are evaluated and the implications for regulation analysis discussed.

MODEL SPECIFICATION: SYSTEMATIC EFFECTS

Specification of Solvent Use

In a very straight forward form, a model for the use of one solvent could be expressed as a linear relation between total use of a solvent and its individual end uses.

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k \quad (4.1)$$

where

y \equiv Total use of a chlorinated solvent,
excluding exports and including imports
(4 main solvents: PERC, METH, TCE, and TCA.
CFC-113 is omitted due to the lack of data.)

X \equiv Index of industrial production for an end use
that uses one or more solvents as inputs.
(k possible end uses)

P \equiv Market price of a chlorinated solvent.

Here the β represent a measure of intensity of the solvent use in the industrial sector X . A model estimated on the above equation, by estimating one value for β , implicitly assumes that the intensity of

solvent use remains constant over time. Since the intensity of use has changed with improved technology and is affected by solvent prices and regulatory actions, the coefficient of the intensity of use, β , will be explicitly modeled as a function of other forces.

$$\beta_i = f(P_{\text{own}}, P_{\text{other}}, \text{Regulatory Pressure, Technological Change}),$$

where P_{own} is the chemical's own price and

P_{other} is the price of substitute chemicals.

Each determinate of the intensity of use will be discussed in turn.

Price Effects. Specifically, the coefficients of the intensity of use, the β 's, are made functionally dependent upon the price of the solvent *relative* to the price of substitute solvents:

$$\beta_1 = \alpha_0 + \alpha_1(P_{\text{own}}/P_{\text{other}}) \quad (4.2)$$

To illustrate what this means in terms of the original solvent use relationship, substitute 4.2 into a simplified version of 4.1

$$y = \beta_0 + \beta_1 X_1$$

to find

$$y = \beta_0 + \alpha_0 X_1 + \alpha_1 [X_1 (P_{\text{own}}/P_{\text{other}})] \quad (4.3)$$

Note that the relative price specification possesses several advantages. The ratio form of prices will control for any constant movement in the prices through time, thus obviating the need to decide upon a price deflator. Any deflator used on the separate prices would cancel out in the ratio form. A relative price can also be interpreted within economic theory as the relevant constraint for the cost minimizing choice of chemical inputs with capital/output ratios fixed in the short-run. A very powerful statistical advantage of the relative price specification lies in the reduction of the number of parameters requiring estimation. Given the limited history contained in the Chlorinated Solvents Data Base, model parsimony would be a strong argument for the use of relative prices.

Identification of Price Effects

The measures of price enter into the equation for solvent use as fixed values, exogenously determined. If instead prices are also codetermined by many of the same forces acting upon solvent use, the estimates of price effects will be confounded. In econometrics, this is known as the identification problem--one has not identified the effects one wishes to measure. For example, if the system of equations does not control for changes in the cost factors, a shift in a supply curve may be mistaken for a movement along a demand curve. If prices are determined within the system and the model ignores this codetermination, then bias is induced in the estimate of a price effect. This is known as "endogeneity bias."

Fortunately the specification of exogenously determined price measures can be empirically tested using a specification test proposed by Hausman (1978). To test the endogeneity of a set of variables in a regression equation, one needs to find a set of instruments correlated with the possibly endogenous variables, yet uncorrelated with the original regression error. In our case the constructed measure of the marginal feedstock cost for a particular solvent and its substitutes can serve as instruments for the price of that solvent. Since the marginal feedstock costs are uncorrelated with the solvent use error term, endogeneity will induce no bias in the estimates of their coefficients.

The Hausman test compares two types of estimators in an expanded regression framework--efficient estimators and consistent estimators. The first type assume that the explanatory variables are orthogonal to the error term for efficiency gains. If this hypothesis proves false, these efficient estimators are biased. The second type of estimator makes no assumption regarding the relationship of the explanatory variables to the error terms and, hence, remains a consistent estimator.

In the present case, a least squares (LS) estimator will be both consistent and asymptotically efficient under the null hypothesis that the price measures are exogenous but will be inconsistent under the alternative hypothesis. The instrumental variable estimators, β_{IV} , will be consistent under both null and alternative hypotheses but will not be

asymptotically efficient if the price measures are exogenous. Under the null hypothesis of exogeneity, the difference between the residuals of the two equations has a probability limit of zero, whereas under the alternative hypothesis the estimates will be different.

Applied to the use of chlorinated solvents, a Hausman test was used to test for the endogeneity of the relative price measures. The test was conducted by first estimating the solvent use function (4.3) using LS and then reestimating the equation substituting the prediction from the equation containing the marginal feedstock cost instruments, labeled MC. Since prediction is the main objective of the instrumental equation, the most unrestricted functional form was used. Illustrating using the simple case of TCA, the following equations apply:

$$y_{tca} = \beta_0 + \alpha_1 X_{metal} + \alpha_2 [X_{metal} (P_{tca}/P_{tce})]$$

where

$$[X_{metal} (P_{tca}/P_{tce})] = \gamma_0 + \gamma_1 X_{metal} + \gamma_2 MC_{tca} + \gamma_3 MC_{tce}$$

If the price measures are uncorrelated with the regression error

$E(\hat{\alpha}_{2,ls}) = E(\hat{\alpha}_{2,iv})$. The results of the Hausman Test regressions are shown in Table 3. The calculated Hausman's test statistic is 3.745, which exceeds the critical value of χ^2 at the 10% level of significance of 2.706 with one degree of freedom. Thus the null hypothesis of exogeneity of price measures is rejected, implying the need for the alternative specification of total solvent use.

Regulatory Pressure and Technological Change

In a statistical sense, it will be hard to separate the effects of technological change from those of regulatory pressure. New government regulations often bring about or hasten technological change. Since their effects tend to be intermingled, they will be discussed together.

Table 3

HAUSMAN TEST, TCA USE
SINGLE EQUATION FOR HAUSMAN TEST FOR ENDOGENOUS PRICES

VARIABLE	LS	IV
INTERCEPT	-37084.59 (6950.76)	-30601.28 (8278.24)
METAL CLEANING INDEX	1527.33 (108.26)	1814.51 (186.78)
INTERACTION OF METAL CLEANING INDEX AND RELATIVE PRIDE OF TCA TO TCE	-373.00 (80.73)	-651.70 (165.70)
WINTER DUMMY VARIABLE	-3243.52 (2385.62)	-3314.37 (2612.04)
SPRING DUMMY VARIABLE	-5664.60 (2382.66)	-5662.42 (2608.55)
SUMER DUMMY VARIABLE	-1391.79 (2423.55)	-1463.52 (2653.56)
	0.820	0.801
	1.122	0.960

Note: Standard errors are in parentheses.

As it stands in the model presented above, the effect of regulation and technology are not explicitly considered. To better understand how regulation influenced use, one would need to include measures of regulation in the modeling. In a univariate sense, a single measure of regulatory pressure for each chemical might suffice. Unfortunately, it would be extremely difficult to avoid subjectivity in the derivation of a formal measure.

If the characteristics of regulation were handled in a multivariate form, one could specify a vector r for each time period. Each element of r would represent an objective measure of a characteristic of regulation: amount of production capability under local regulation, amount of production under binding TLVs in the workplace, required workplace controls, etc. The construction of a meaningful multivariate measure of regulatory pressure may be no less subjective than the univariate measure.

Left with no direct measure of regulation, the systematic effects of regulation over time can only be measured by adding functions of calendar time to the variables explaining the β 's. These variables then act as surrogates for all unknown time related forces affecting the β 's. Its validity is limited by the closeness of the unknown dynamic force to the specified function of calendar time. The validity of these measures and other issues in the estimation of a proxy for regulatory pressure are addressed in the section titled "Estimation Results."

As an alternative to the systemwide estimation of dynamic time effects, a different approach is also taken. The effects of regulation are documented by estimating the system of equations over a period without substantial regulation. Projections from the "market" capturing only market forces are compared to the actual use of solvents under regulations to show the effect of regulatory pressure.

MODEL SPECIFICATION: ERROR STRUCTURE

The systematic portion of a model of chlorinated solvent use has been specified

$$y_{it} = f(Z_{it}; \beta) + e_{it}$$

where y is solvent use, Z is a set of explanatory variables, and β is the set of coefficients to be estimated. I now specify a structure for the error covariance matrix, $E(e, e') = \Omega$. The data will be ordered by the index for the solvent $i = 1 \dots M$ and the index for time $t = 1 \dots T$. Four solvents are being modeled ($M=4$) and the length of the time period will vary.

We make the following assumptions about the error terms e_{it} :

First-order autocorrelation. The stochastic influences on solvent use are likely to be related over calendar time. To allow for correlation of disturbances over time, assume that the error term is generated by a stationary, first-order autoregressive [AR(1)] process

$$e_{it} = \rho_{ii}e_{i,t-1} + \varepsilon_{it}$$

so that the value of the error term depends on its previous value.

Zero Mean. $E(\varepsilon_{it}) = 0$ for all i, t .

Homoskedastic Variance. $E(\varepsilon_{it}, \varepsilon_{jt}) = \sigma_{ij}$ for all i, j, t .

Contemporaneous Covariance. The different chlorinated solvents are subject to many of the same stochastic influences. For instance the effects of weather or even the political climate may be similar for all solvents. Hence correlated disturbances are allowed across solvents for a given time period, i.e., σ_{ij} is nonzero for $i \neq j$.

These assumptions about the error structure were not chosen arbitrarily; alternatives to these assumptions were considered and tested for empirically. These alternatives are discussed below. Appendix D analytically derives the implications of the above assumptions for the error covariance matrix and sets forth an estimation procedure embodying these implications in a series of sequential steps. This estimation procedure combines a correction for autocorrelation with allowance for contemporaneous correlation to yield an approximate estimated general least squares (EGLS) estimator¹.

Time Structure: Estimates of longer autoregressive orders were also made and plotted in the form of correlograms. The choice of the exact

¹The estimation procedure of Appendix D outlines a two-step approximate EGLS estimator that guarantees convergence. Various maximum likelihood estimators were also experimented with. The convergence of these estimators is unstable for some equations, depending on the proxy used to represent regulatory effects. Hence, only the more straightforward EGLS results are presented in the text.

length of the autoregressive order turned on the more formal method of Hiaso (1982). This method uses an information criterion developed by Akaike, called the final prediction error (FPE) that is defined as:

$$\text{FPE} = \frac{(T + N + M + 1)}{(T - N - M - 1)} \cdot \frac{\sum (Y_t - \hat{Y}_t)^2}{T}$$

where T is the number of observations, N is the number of systematic parameters, and M is the number of autoregressive parameters. This criterion incorporates a measure of model fit (sum of squared prediction error) that is weighted by a multiplicative term to account for the number of parameters used to obtain the fit. Thus, the FPE criterion reflects the fundamental tradeoff in modeling between the tightness of fit and model parsimony. Models were estimated for autoregressive orders ranging from zero to four, the associated FPE statistic calculated, and the model having the lowest FPE was chosen as the best tradeoff between fit and parsimony.

In general, the FPE criterion would always select the first order autoregressive specification. Correlagrams were also plotted from the estimated autocorrelation function of the computed model errors and used as a diagnostic check.

An alternative specification of the time structure would have the value of the error term dependent upon the lagged values of the error terms in all equations. This is referred to as a "vector autoregressive," or VAR, model. For situations where the number of equations is greater than two and the number of observations is limited, Monte Carlo studies suggest difficulty in obtaining precise estimates of the autoregressive parameters of a VAR error term². This was borne out with this data set by the exploratory work done with the assumption of VAR errors. VAR models were estimated and rejected based upon the FPE criterion--the small improvement in prediction was more than offset by the lost degrees of freedom for the additional autoregressive parameters.

² For example, Doran and Griffiths (1983), using a three equation model with twenty observations, found the assumption of single equation AR(1) errors to produce better estimates even when the assumption was not true.

Heteroskedasticity: The hypothesis of a nonconstant variance through time was considered and tested by means of a test proposed by Breusch and Pagan (1979) based on the residuals of the regression equation. The Breusch-Pagan test indicated that the hypothesis could be rejected at a high level of confidence.

THE CHLORINATED SOLVENTS DATA BASE

Total Solvent Use

The model of chlorinated solvents will use the production values rather than the sales data as the dependent variable for several reasons. First, the production and sales data tend to move very closely together, lending weight to the assertion that the solvents, bulky and costly to store, do not stay long in inventory. Hence there should be no discrepancy due to stockpiling. Second, the International Trade Commission (ITC) report the production of solvents each month, making possible a higher degree of precision in parameter estimation. The last argument in favor of using production data is that sales data can omit transactions internal to one chemical plant. In the incestuous world of chemical production, the output of one process may be the input to another within the same production facility. Such a transaction would be captured in the ITC production figure and omitted in a sales figure.

Aggregate domestic production data could still be a poor proxy for domestic use since it includes the fraction destined for export and makes no account for the amount that is imported for domestic use. The proxy for the total domestic use of solvents will subtract out exports and add in imports to the production quantities reported by the ITC. This will yield the appropriate "left-hand side" variable and the only modeling question that remains relates to how the level of imports and exports can influence the determinates of solvent use--mainly, chemical prices. Since international trade can obviously influence the prices in domestic markets, measures of trade will be included in the instrumental equations for chemical prices.

Variable Names: The dependent variable for the use of a chlorinated solvent--production quantity minus exports plus imports--is designated using the chemical abbreviations used throughout this document. They are:

PERC_PU	PERC Proxy of Use, PERC_PQ - Exports + Imports,
METH_PU	METH Proxy of Use, METH_PQ - Exports + Imports,
TCE_PU	TCE Proxy of Use, TCE_PQ - Exports + Imports, and
TCA_RU	TCA Proxy of Use, TCA_PQ (Trade data not reported).

Solvent Prices

List prices for the chemical solvents, though available from the *Chemical Marketing Reporter*, were not used because they do not measure the transactions that occur in the market. In general, the list price for a chemical will not reveal the extent of discounting by distributors or reflect changes in the units in which the solvent is purchased. The perchloroethylene list price, for example, increased throughout 1966 even though the average purchase price declined as a result of a general increase in bulk purchases. To arrive at a better measure of the market transaction price, an "average" selling price (unit value) may be imputed by dividing the total sales revenue by the total sales quantity. Using data from the ITC, average sales prices were constructed and compared with list prices. The simple correlation coefficients were, in general, quite high. But when the two measures of price were graphically compared, the list prices tended to exhibit "sticky" behavior that lagged the movement of average sales prices. For these reasons, the imputed sales prices will be used in the estimation of the parameters of the model of chlorinated solvents.

Variable Names: The sales prices of the various chemicals also use the chemical names used throughout this document. In addition, several substitute solvents are added. The following variable names are used:

PERC_SP	PERC Sales Price,
METH_SP	METH Sales Price,
TCE_SP	TCE Sales Price,
TCA_SP	TCA Sales Price,
F11_SP	CFC-11 Sales Price, and
LPG_P	Hydrocarbon Solvent Price Proxy, (Liquid Propane Gas Price)

End Uses

To measure the level of economic activity in the parts of the economy that use chlorinated solvents, several indices of industrial production reported by the Federal Reserve Board are used. Serious problems in mismeasurement of the indices of industrial production are not expected, rather the problem is one of aggregation. How well does the well-measured aggregate index capture the exact sectors of the economy that use chlorinated solvents? To some extent, these indices of economic activity will remain imperfect measures: they will include some activities that do not pertain to solvent use and exclude activities that do. Careful selection of indices can decrease the divergence. The indices come largely from series published monthly in the Federal Reserve statistical release, "G.12.3: Industrial Production."

Variable Names: In general the indices of industrial production in sectors of the economy that use chlorinated solvents are expressed in five character variable names. Hence, the index of sectors using solvents in metal cleaning is named METDX. The names are:

METDX	Metal Cleaning Index, SIC 252 34 36 37 39
KNITS	Knit Garments, SIC 2253,4,7-9
PAINT	Paint End Uses, SIC 2850
FBLow	CFC-11 Subst. Uses: Blown foams (RAND est.) and Aerosols (Use Metal Can Index as proxy, SIC 3411)

The Interaction of End Uses with Relative Prices

The model is specified so that that prices affect use only through an individual end use sector. Individual price effects have the nonsensical interpretation of having a direct effect on use independent of the level of economic activity. Hence the model requires that price effects occur through particular end use sectors. This indirect effect is portrayed through an interaction term--the multiplication of the indice of end use by the relative price measure. This constructed variable is then used as the dependent variable in an instrumental equation using all the exogenous variables in the model. The predicted values from the instrumental equations are then used in place of the original values in the use equations.

Variable Names: The interaction term will begin with the first three characters of the index variable name. For instance, the interaction term of the metal cleaning index and its relative price measure would be: MET_RP. (An additional letter is attached to the variable name to indicate to which chemical market the relative price relates.) The names are:

MET_PRP	Interaction of $\text{METDX} * \text{PERC_SP} / ((\text{TCA_SP} + \text{TCE_SP}) / 2)$,
MET_MRP	Interaction of $\text{METDX} * \text{METH_SP} / ((\text{TCA_SP} + \text{TCE_SP}) / 2)$,
PAI_MRP	Interaction of $\text{PAINT} * \text{METH_SP} / \text{LPG_P}$,
FBL_MRP	Interaction of $\text{FBLOW} * \text{METH_SP} / \text{CFC-11_SP}$,
MET_ERP	Interaction of $\text{METDX} * \text{TCE_SP} / \text{TCA_SP}$, and
MET_ARP	Interaction of $\text{METDX} * \text{TCA_SP} / \text{TCE_SP}$.

The Model for Chlorinated Solvents

Table 4 contains the specification of the complete multiple equation chlorinated solvents model using the variable names given above. Do note that the instrumental values are used for the interaction term--i.e., the projection of the interaction term on all the exogenous variables, including marginal feedstock costs. In addition to the systematic terms below, quarterly dummy variables will be introduced to capture any constant seasonal component.

Table 4

THE SPECIFICATION OF THE MODEL FOR CHLORINATED SOLVENTS

$$\text{PERC_PU} = \beta_{10} + \beta_{11} \text{METDX} + \beta_{12} \text{KNITS} + \alpha_1 \text{MET_PRP_};$$

$$\begin{aligned} \text{METH_PU} = & \beta_{20} + \beta_{21} \text{METDX} + \beta_{22} \text{PAINT} + \beta_{23} \text{FBLOW} \\ & + \alpha_{21} \text{MET_MRP_} + \alpha_{22} \text{PAI_MRP_} + \alpha_{23} \text{FBL_MRP_}; \end{aligned}$$

$$\text{TCE_PU} = \beta_{30} + \beta_{31} \text{METDX} + \alpha_{31} \text{MET_ERP_};$$

$$\text{TCA_RU} = \beta_{40} + \beta_{41} \text{METDX} + \alpha_{41} \text{MET_ARP_};$$

ESTIMATION RESULTS

The estimation results will be presented in two parts to address the difficulty of isolating and measuring the effect of regulation on the markets for chlorinated solvents. First, the effects of regulation will be documented and presented graphically using the chlorinated solvents model in a form of "intervention analysis." Then the model will be reestimated using deterministic functions of calendar time to attempt to capture the effect of regulation.

Documenting the Effects of Regulation

A strategy derived from time series literature is used to document the effect of regulation. Pioneered by Box and Tiao (1965, 1973, and 1975), "intervention analysis" seeks to measure the nature and magnitude of the change brought about by a known intervention.³ It differs from the classic statistical tests for changes in mean by taking into account the time series structure contained in the observations. A Student's *t* test, for example, assumes that observations before and after the event have constant means, μ_1 and μ_2 , and are distributed normally, with

³This term was introduced by Glass (1972) based on earlier work in Box and Tiao (1965). It denotes a nonstochastic shift, known *a priori*, that affects a possibly nonstationary time series.

constant variance, and independently. When the observations come from a time series, serial dependence is likely in addition to the possibility of nonstationarity and seasonal effects. Hence, the classical parametric procedures that rely on independence are not strictly valid. Instead, a stochastic model that accounts for these time dependent effects and then used to estimate the magnitude of the intervention.

Intervention analysis can be used to document the effects of regulation upon the markets for chlorinated solvents. The outside "intervention" is obviously that of government regulations placed on solvents. Hence, a model for use of a chlorinated solvent, that also accounts for the time series structure of solvent use, is estimated over a period of time where government regulation or technical change was negligible. This model then captures only the effects of market forces. This market model is then projected forward into a period where government intervention or technical change increased. The predictions from the market models are counterfactual in that they state what would have happened if no government intervention had occurred. This is known not to be true. The difference between the counterfactual predictions of use from the market model and the factual use shows the effects of those forces excluded from the market model: regulatory and technical change. Thus, one can formulate the hypothesis that the divergence will be less for those solvents having a history of relatively little regulation (METH and TCA). Conversely, those solvents having a history of relatively high regulatory pressure (PERC and TCE) will exhibit a large divergence between use predicted by a market model and actual use.⁴

A Simple Model. To demonstrate the idea of intervention analysis a single equation model for TCE will be used because of its rich and complex regulatory history. In general an early section of the data is chosen to represent the period with little regulatory activity. The model presented below was estimated on the first five years of data from 1965 to 1970.

⁴More complicated conjectures can be made based upon interactions among the chemicals. The fact that the less regulated (METH and TCA) were substituted for the more regulated (PERC and TCE) would also lessen the expected divergence caused by regulation of METH & TCA.

$$y_{tce} = 17188 + 94 X_{\text{metal cleaning}} - 56 \left[X_{\text{metal cleaning}} z \left(\frac{P_{tce}}{P_{tca}} \right) \right]$$

$$- 1154 \text{ Winter} + 398 \text{ Summer} - 1567 \text{ Fall}$$

This model is used to make unconditional forecasts beyond the sample period (with little regulation) into the later period (with considerable regulation). Figure 3 plots the model predictions (squares) and the actual values (circles) against time. This model manifests great disparity between the predicted values (absent regulatory intervention) and the actual values (under regulatory intervention). The model suggests that absent outside intervention, the market for TCE would have experienced continued moderate growth. This did not occur because the market responded to the intervention of government regulations put upon TCE.⁵

Multiple Equation Model: The single equation model of TCE ignores the interactions with the markets for other substitute chemicals. The approximate generalized least squares estimates for the market model (1965-1975) are shown in Table 5)⁶.

⁵Models that omit the regulatory intervention will have biased parameter estimates and degraded forecasts.

⁶A sample SAS program of the multiple equation estimation procedure is contained in Appendix E. Missing production values for METH in the early years and TCE in the later years were substituted with predictions from autoregressive single equation models so that these years would be available for estimation of the entire system. The use of predicted values for these years, it is argued, keeps the information set available for estimation as large as possible. Results are not qualitatively different from the results based on data that omits any time point with one missing value.

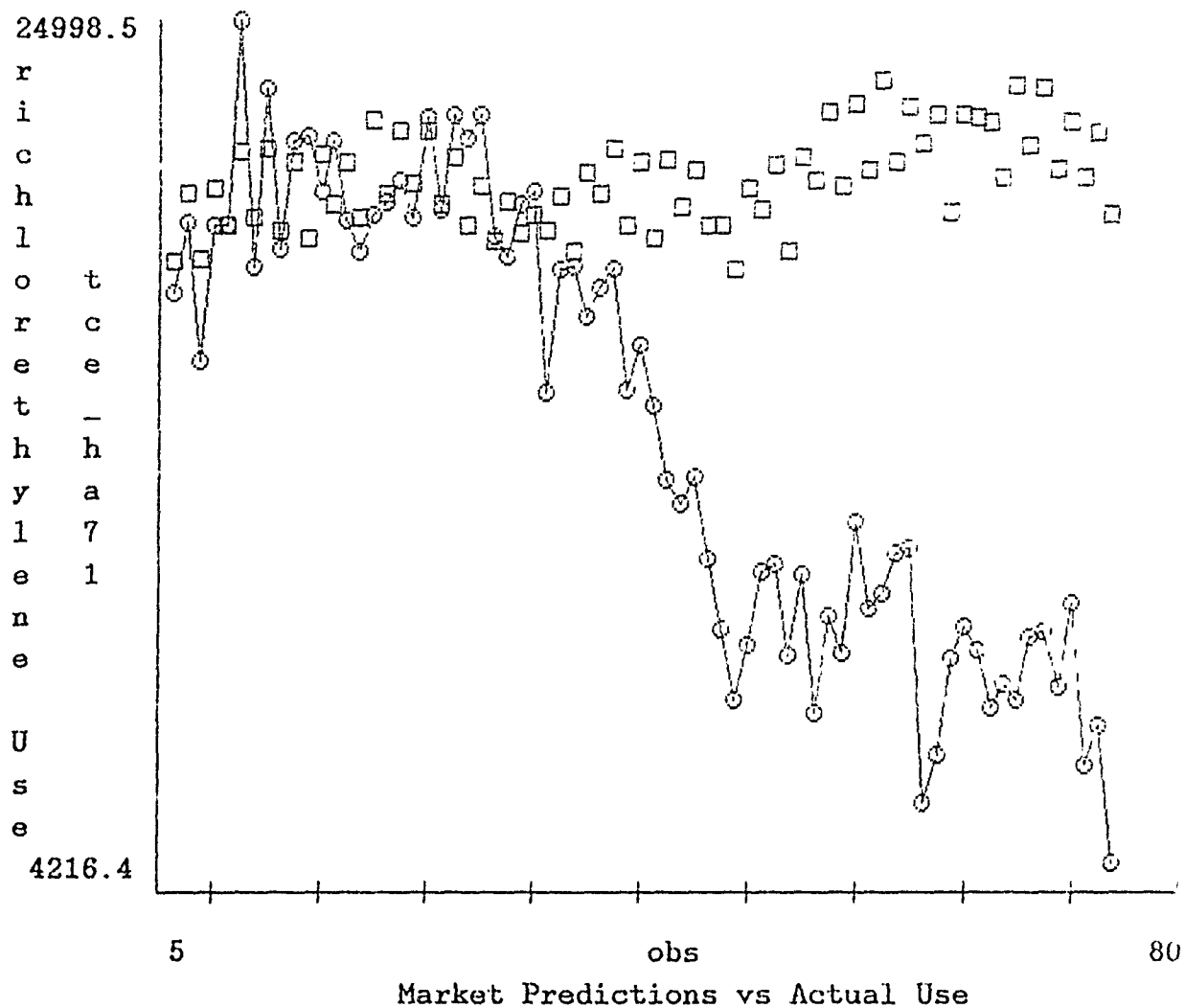


Figure 3: TCE Single Equation Model

Table 5

MARKET MODEL ESTIMATES, 1965-1975
APPROXIMATE GLS - SEEMINGLY UNRELATED REGRESSION WITH AR(1) CORRECTION

Variable	Coefficient	Std. Error	Variable Label
Equation 1: PERC_PU			
P_BETA0	16509.04	5167.96	Intercept
P_METDX	-48.17	363.16	Metal Cleaning Index
KNITS	-146.18	179.75	Knit Garments
MET_PRP_	288.45	111.95	Rel. Price Interaction for METDX
P_Q1	-996.20	1926.23	Winter Quarter
P_Q2	-3997.73	1775.20	Summer Quarter
P_Q3	-3081.59	2666.43	Fall Quarter
Equation 2: METH_PU			
M_BETA0	-20907.68	12401.63	Intercept
M_METDX	423.07	291.67	Metal Cleaning Index
PAINT	285.29	315.37	Paint End Uses
FBLow	30.08	428.62	CFC-11 Subst. Uses
MET_MRP_	-119.96	147.41	Rel. Price Interaction for METDX
PAI_MRP_	-79.67	81.77	Rel. Price Interaction for PAINT
FBL_MRP_	909.55	806.77	Rel. Price Interaction for FBLow
M_Q1	-3879.82	2630.81	Winter Quarter
M_Q2	-9901.05	4984.22	Summer Quarter
M_Q3	-6834.76	4260.76	Fall Quarter
Equation 3: TCE_PU			
E_BETA0	8624.73	2852.61	Intercept
E_METDX	-73.95	114.52	Metal Cleaning Index
MET_ERP_	-58.26	47.18	Rel. Price Interaction for METDX
E_Q1	-1240.29	731.51	Winter Quarter
E_Q2	-275.50	797.86	Summer Quarter
E_Q3	-1187.43	744.01	Fall Quarter
Equation 4: TCA_RL			
A_BETA0	-6877.28	12562.59	Intercept
A_METDX	1245.64	261.54	Metal Cleaning Index
MET_ARP_	-387.04	134.15	Rel. Price Interaction for METDX
A_Q1	-2544.78	2564.98	Winter Quarter
A_Q2	-5798.75	2750.09	Summer Quarter
A_Q3	-2440.45	2544.17	Fall Quarter

The comparison of predicted values (market effects, no regulatory effects) and actual values (market and regulatory effects) follow in Figures 4 through 7.⁷ The predicted values of the market model continue beyond the period over which the model was estimated. The comparison of interest lies between the predictions of the market model and the actual values after 1975.

Figure 4 shows this type of plot for the approximate GLS model for TCE over the years 1965-1975. Since the 1965-1975 period leaves very few points representing "little regulatory activity" for TCE, no systematic divergence between the predictions and the actual values exist. This should not surprise; the market model for TCE also captures nonmarket forces.

Figure 5--showing the comparison for PERC--is striking in the extent to which it exhibits a great disparity between the prediction of market forces and the reality of chemical production. The uncaptured effect of regulatory pressure, with associated changes in technology, brings about much of this great divergence. Briefly, users of PERC shifted to more efficient equipment in what may be termed an anticipatory reaction to the threat of regulation.⁸

Figures 6 and 7--showing the comparisons for TCA and METH-- reveal a different story. The contrast between the predictions of the market model and the actual levels of production confirm the conclusion gleaned from the technical analysis: TCA and METH have not witnessed broad regulatory effects. On the contrary, both markets have been augmented

⁷Please note that Figures 4 through 7 plot the predicted and actual values in terms of the Z^* transformed matrix. The transformation subtracts a fraction of the previous period's value, the fraction determined by the estimated $\hat{\rho}$. If $\hat{\rho}$ equals one, the differences between levels are used and if $\hat{\rho}$ equals zero, the levels alone are used. To derive predictions in terms of the original Z values from a model with serially correlated error, one may use the following forecasting formula:

$$y_{t+1} = \hat{\rho} y_t + \beta(1-\hat{\rho}) + \beta (X_{t+1} - \hat{\rho} X_t)$$

⁸A more thorough explanation of the regulatory history of PERC markets can be found in Wolf and Myers (1987).

SEEMINGLY UNRELATED REGRESSION W AR(1) - 67 TO 75

PLOT OF TCE_PU*DATE
PLOT OF EHAT*DATE

LEGEND: A = 1 OBS
SYMBOL USED IS *

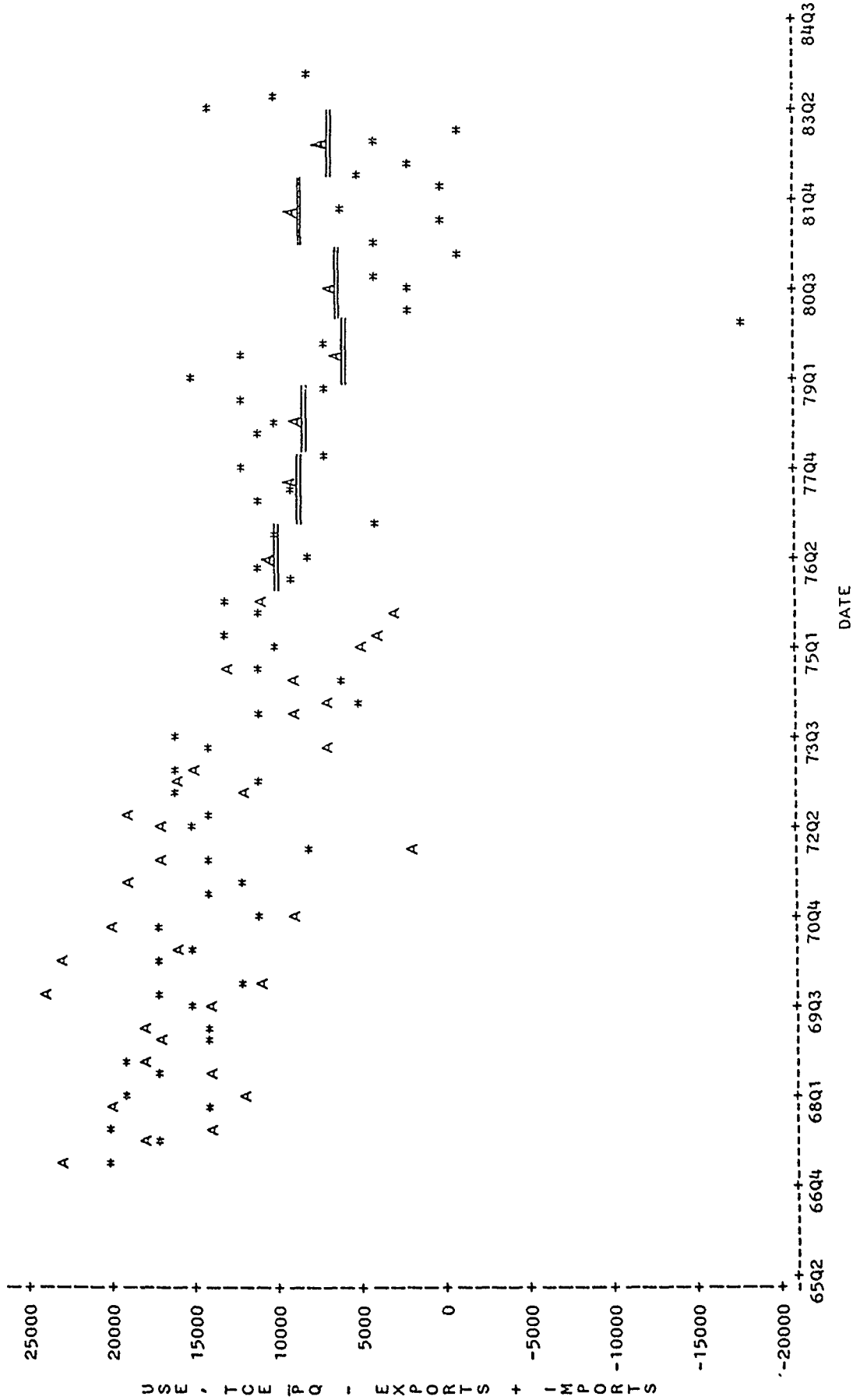


Fig 4

TCE Market Model: Predictions versus Actual

SEEMINGLY UNRELATED REGRESSION W AR(1) - 67 TO 75

PLOT OF PERC_PU*DATE
PLOT OF PHAT*DATE

LEGEND: A = 1 OBS
SYMBOL USED IS *

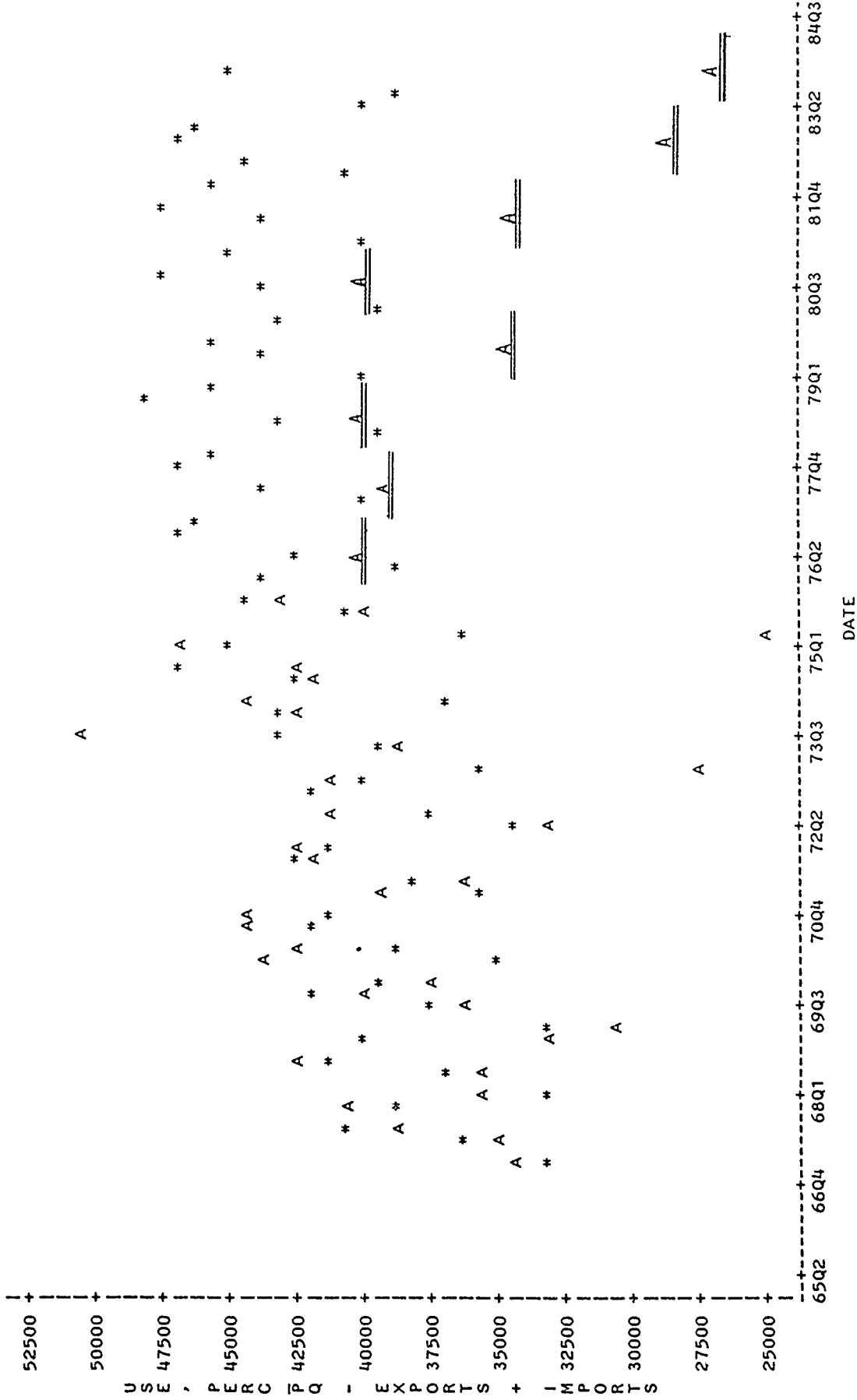


Fig 5
PERC Market Model: Predictions versus Actual

SEEMINGLY UNRELATED REGRESSION W AR(1) - 67 TO 75

PLOT OF TCA_RU*DATE
 PLOT OF AHAT*DATE
 LEGEND: A = 1 OBS
 SYMBOL USED IS *

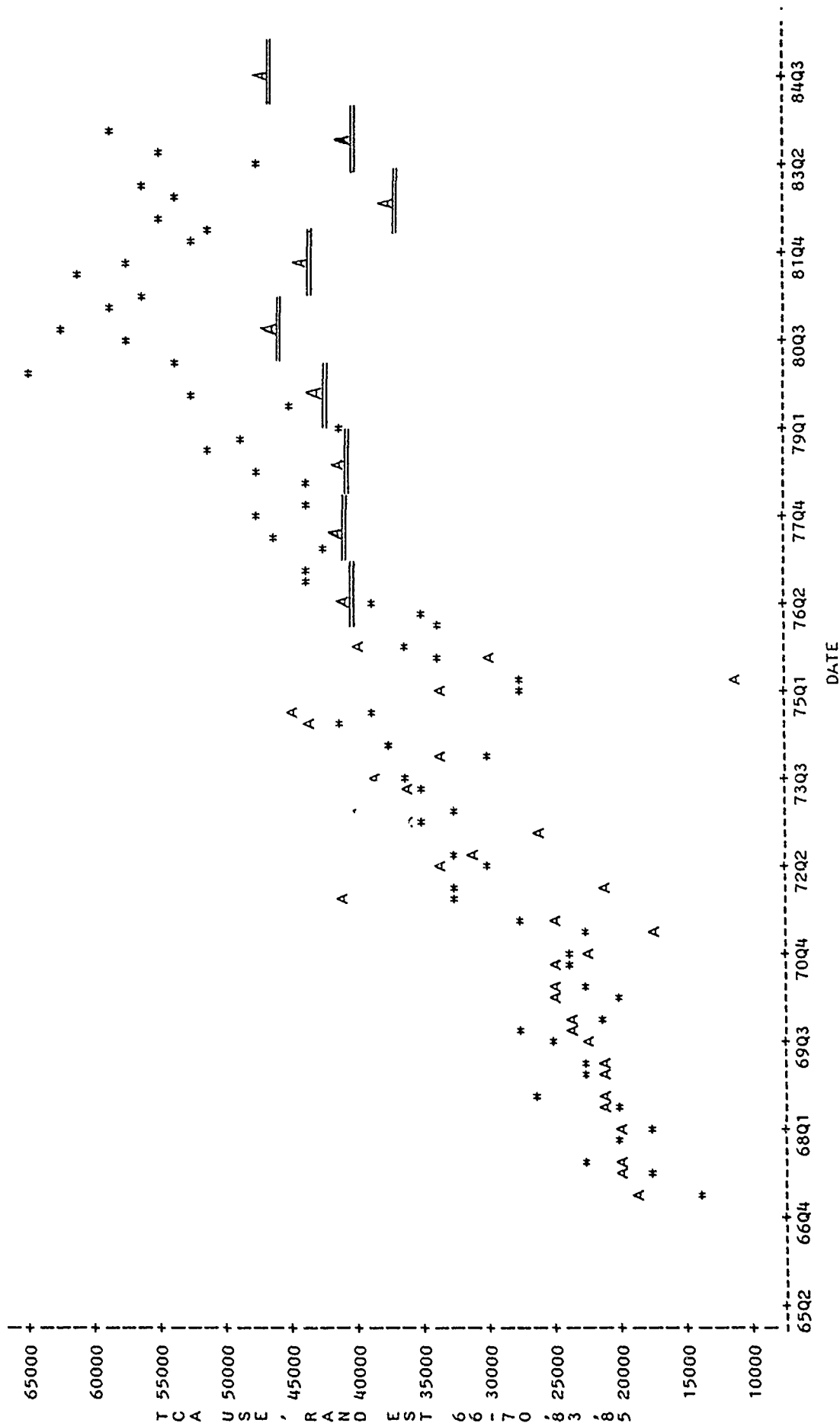


Fig 6

TCA Market Model: Predictions versus Actual

SEEMINGLY UNRELATED REGRESSION W AR(1) - 67 TO 75

PLOT OF METH_PU*DATE
 PLOT OF MHAT*DATE
 LEGEND: A = 1 OBS
 SYMBOL USED IS *

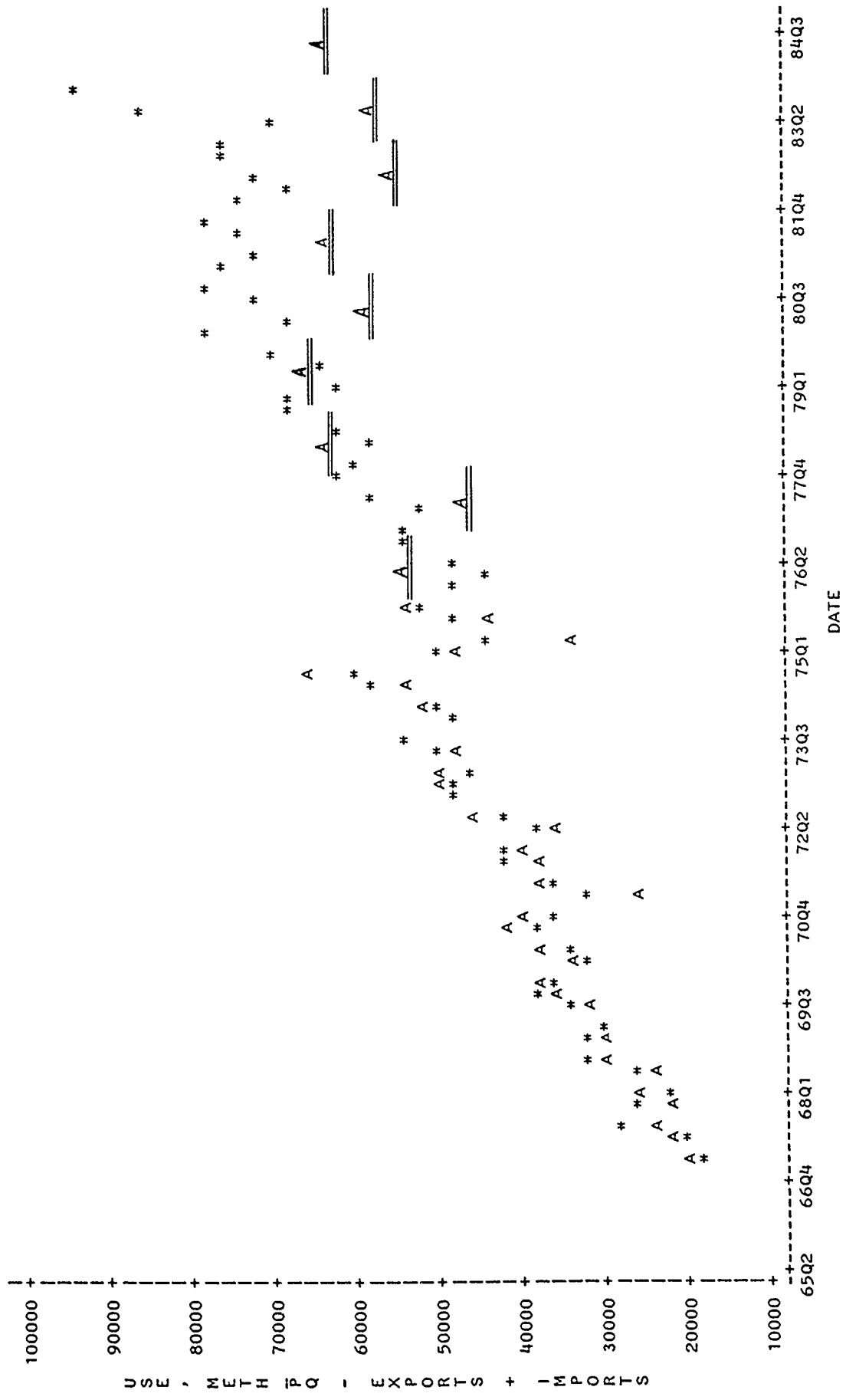


Fig 7
 METH Market Model: Predictions versus Actual

by customers driven from other markets by regulation or the threat of regulation. This is not to say that the market model predicts perfectly; the later years still reveal some outside effect not captured by the market model. Even though the forecast error grows with increasing forecast length, both of these models could be improved with better specification of regulatory forces.

Estimating A Proxy for Regulatory Pressure

The market model presented above excludes the effect of regulation. In terms of the statistical theory, the omitted variable of regulation induces bias in the coefficient estimates. Thus no interpretation will be made of these coefficients. To address this problem, one must estimate a proxy for regulatory pressure. The simplest proxy for the effect of regulation might account for a constant shift on the day a regulation came into effect. This is absurd in that it assumes the complete effect of that regulation occurred at that one point in time. To account for an ongoing effect through time, linear time trends will be used.⁹

The lack of a measure of regulation makes the use of dynamic functions of calendar time, even with the associated estimation problems, a lesser evil than the omitted variable bias that occurs when no measure of regulation is used. Linear time trends are used to capture the omitted variable of regulation. Nonlinear dynamic functions are computationally difficult to enact. Appendix F presents exploratory work on specifying and estimating functional forms other than the linear trend presented in the text.

Table 6A and Table 6B compare the estimation procedure with and without the use of trend terms. The coefficients of the complete model in these tables should be compared to reasonable *a priori* expectations. One should expect higher levels of solvent use when economic activity

⁹Though conceptually straight forward, the use of trend terms can make for problematic estimation. In order for this specification to be valid, the series must be stationary about a deterministic trend. If this is not the case, as is pointed out by Nelson and Kang (1984), then the standard statistical inference will not hold.

using that solvent increases. Thus, the coefficient on the level of economic activity is expected to be positive. The coefficient on the relative price measure, on the other hand, should be negative if one expects that solvent use to vary inversely with its price. Exceptions exist to both of theoretical expectations. The most important exception concerns the sign of the coefficient on the relative price measure. During periods of regulatory pressure, one may reasonably expect the price and the use of a solvent to decrease. Correspondingly, the use of substitutes to the regulated solvent may increase at the same time they are becoming relatively more expensive.

Table 6A

COMPLETE MODEL ESTIMATES, 1965-1983
APPROXIMATE GLS - SEEMINGLY UNRELATED REGRESSION WITH AR(1) CORRECTION

Variable	Coefficient No Trend	Coefficient With Trend	Variable Label
Equation 1: PERC_PU			
P_BETA0	26605.39 (5.62)	19536.51 (2.59)	Intercept
P_METDX	-432.62 (-2.58)	-113.55 (-0.42)	Metal Cleaning Index
KNITS	339.08 (2.96)	316.59 (2.67)	Knit Garments
MET_PRP_	188.62 (2.16)	156.21 (1.80)	Rel. Price Interaction for METDX
P_Q1	-1927.75 (-1.12)	-1389.74 (-0.80)	Winter Quarter
P_Q2	-9583.82 (-5.25)	-8696.09 (-4.41)	Summer Quarter
P_Q3	-10115.43 (-4.96)	-8582.06 (-3.54)	Fall Quarter
KNI_T74		-14.35 (-1.57)	KNITS * Trend_70
Equation 2: METH_PU			
M_BETA0	-27153.94 (-2.99)	-25680.97 (-2.82)	Intercept
M_METDX	457.83 (2.12)	429.28 (1.98)	Metal Cleaning Index
PAINT	-177.59 (-1.14)	-217.17 (-1.38)	Paint End Uses
FBLOW	691.48 (3.79)	733.24 (3.98)	CFC-11 Subst. Uses
MET_MRP_	-80.42 (-0.78)	-85.60 (-0.83)	Rel. Price Interaction for METDX
PAI_MRP_	88.54 (2.22)	101.75 (2.52)	Rel. Price Interaction for PAINT
FBL_MRP_	-378.90 (-1.24)	-418.74 (-1.37)	Rel. Price Interaction for FBLOW
M_Q1	-1402.22 (-0.69)	-1403.28 (-0.69)	Winter Quarter
M_Q2	-7156.91 (-1.74)	-7147.47 (-1.73)	Summer Quarter
M_Q3	-5718.64 (-1.77)	-5791.55 (-1.79)	Fall Quarter

Note: Students' *t* based on asymptotic standard error in parentheses

Table 6B

COMPLETE MODEL ESTIMATES, 1965-1983
APPROXIMATE GLS - SEEMINGLY UNRELATED REGRESSION WITH AR(1) CORRECTION

Equation 3: TCE_PU

E_BETA0	20463.24 (11.38)	5452.17 (2.32)	Intercept
E_METDX	-280.45 (-5.94)	147.00 (2.24)	Metal Cleaning Index
MET_ERP_	-67.95 (-1.91)	-45.47 (-1.73)	Rel. Price Interaction for METDX
E_Q1	-1939.00 (-3.27)	-718.96 (-1.54)	Winter Quarter
E_Q2	-706.45 (-1.06)	12.03 (0.02)	Summer Quarter
E_Q3	-2074.55 (-3.54)	-956.79 (-2.09)	Fall Quarter
MET_T70		-13.36 (-7.76)	METDX * Trend_70

Equation 4: TCA_RU

A_BETA0	-23977.98 (-5.09)	-9751.29 (-1.10)	Intercept
A_METDX	1565.83 (11.55)	1238.07 (6.37)	Metal Cleaning Index
MET_ARP_	-363.57 (-4.59)	-383.79 (-5.33)	Rel. Price Interaction for METDX
A_Q1	-3397.45 (-2.08)	-4390.02 (-2.60)	Winter Quarter
A_Q2	-5707.44 (-3.16)	-6382.43 (-3.51)	Summer Quarter
A_Q3	-1990.54 (-1.23)	-2955.34 (-1.77)	Fall Quarter
MET_T70	10.58 (2.38)		METDX * Trend_70

Note: Students' t based on asymptotic standard error in parentheses

In the PERC equations the signs of the metal cleaning coefficients are opposite that expected. Metal cleaning uses form a small (less than 10 percent) portion of the end uses for PERC, making the influence of

this sector perhaps harder to identify. In any case, the PERC equation that omits any measure of regulatory events is distinctly unsatisfactory, suggesting that these contrary effects are distinguishable from zero.

The addition of a trend term for the sector representing dry cleaning uses (KNITS) leaves the coefficient for the metal cleaning sector indistinguishable from zero. It also indicates a negative trend in the intensity of PERC use for dry cleaning due to concern over possible toxic side effects. Though this is an improvement, the use of a trend term has hardly "solved" the problem of measuring the market relationships. Both PERC equations also exhibit much more seasonality than the equations for the other chemicals.

The METH equation is one of the most complicated because of the wide number of uses. The regulatory pressures upon METH are also less straightforward; none of the trend terms estimated were distinguishable from zero. Hence they are omitted. Of the other coefficients in this equation, the interaction term for the PAINTS sector is positive, reflecting the increased use of METH in paint removers in a time of increasing relative price of METH. This discloses the influence of some of the regulations placed on hydrocarbon alternatives. The lack of a measure for these substitutes precludes capturing this regulatory effect and is a shortcoming of the model. The coefficient on the METH and CFC-11 interaction term do reveal the new demand for METH resulting from increasing prices for CFC-11. This coefficient, however, overstates price effect because of the omitted influence of the regulatory ban on CFC-11 in aerosol use. The model estimates for the METH markets are the least satisfactory. The following subsection, "Evaluation of Model Estimates," will further explore this issue and suggest improved estimates of the market parameters.

The first equation for TCE suggests a negative sector effect. This is due to the omitted effect of the extreme regulatory pressure experienced by TCE markets after 1969. When a trend term is included, the coefficient on the metal cleaning sector matches the *a priori* expectation of a positive sector effect. The price effect agrees with *a priori* expectations in both cases. The estimate of a price effect in

the second model should be more accurate due to the bias in the first model of the omitted regulatory effect.

The equation for TCA shows both strong price effects and strong sector effects. The addition of a trend term does capture the increased intensity of use of TCA due to regulatory pressure upon TCE, but produces no distinguishable change in the other coefficient estimates.

The plausibility of the magnitudes of all the price coefficient estimates are discussed next.

Elasticities. Estimates for the elasticities may also be derived in the above models. These are important in that they provide a measure of the magnitude of price effects among related solvents.

The estimates of mean elasticities derive from the definition of an elasticity as the partial derivative of the y equation with respect to the independent variable X times their ratio. The derivation of the estimate of partial derivatives in the chlorinated solvents model is somewhat more complicated by the interaction term involving the index of industrial production and the relative price measure. The estimate of the partial derivative of use with respect to price will involve the estimated coefficient on the instrument, α , and all terms in the instrument excluding the price term. This is then multiplied times the ratio of price to use taken at the sample means to yield the mean price elasticity.¹⁰

¹⁰Technically speaking, the above generalization is not exactly true. An elasticity is only defined at discrete points in time; any generalization of these elasticities through time, such as a mean, should calculate directly from the estimated point elasticities. This more accurate estimate of a mean elasticity does not, using these data, differ much from more simple estimate given above. (The divergence depends on how far apart in time the mean X and mean Y occur in the sample.) Hence, the more straightforward estimates are presented in this paper.

The other point to note is that the form of the model implies that own price elasticities equate with substitute price elasticities. This result comes naturally from the relative price specification and it accords with Marshall's law of demand requiring the addition of own price elasticities to the weighted sum of cross price elasticities to equal zero.¹¹

¹¹ Rearranging the terms in the definition of an elasticity, the following expression for the elasticity of y with respect to X may be derived:

Elasticity

$$\text{of } y \text{ w.r.t. } X = \varepsilon_{y,X} = \frac{\% \Delta y}{\% \Delta X} = \frac{\partial y / y}{\partial X / X} = \frac{\partial y}{\partial X} \cdot \frac{X}{y}$$

The equation

$$y = \beta^0 + \beta X + \alpha \left[X \left(\frac{P_{\text{own}}}{P_{\text{sub}}} \right) \right]$$

implies the following price elasticities.

The Own Price Elasticity:

$$\varepsilon_{y,P_{\text{own}}} = \frac{\partial y}{\partial P_{\text{own}}} \cdot \left(\frac{P_{\text{own}}}{y} \right) = \left[\alpha \left(\frac{X}{P_{\text{sub}}} \right) \right] \left(\frac{P_{\text{own}}}{y} \right)$$

The Substitute Price Elasticity:

$$\begin{aligned} \varepsilon_{y,P_{\text{sub}}} &= \frac{\partial y}{\partial P_{\text{sub}}} \cdot \left(\frac{P_{\text{sub}}}{y} \right) = \left[-\alpha \left(\frac{X P_{\text{own}}}{P_{\text{sub}}^2} \right) \right] \left(\frac{P_{\text{sub}}}{y} \right) \\ &= -\alpha \left(\frac{X}{P_{\text{sub}}} \right) \left(\frac{P_{\text{own}}}{y} \right) \end{aligned}$$

or

$$\varepsilon_{y,P_{\text{sub}}} = -\varepsilon_{y,P_{\text{own}}}$$

The above result states that the substitute price elasticity is equal in magnitude but opposite in sign to the own price elasticity.

Sector elasticities may also be defined, but are slightly more complicated and yield no easy interpretation since they still depend on the scaling of the sector measure, X .¹²

The estimates of mean elasticities obtained by this technique are presented in Table 7. Only the elasticity estimate for TCA can be discerned from zero with greater than ninety-five percent confidence. Nonetheless, the price elasticity estimates in Table 7 speak to the success achieved by the model of aggregate chemical use for each chlorinated solvent. Both price elasticity estimates for TCE and TCA are negative and in the believably inelastic range, with the TCA market showing slightly more responsiveness to price than the TCE market. The net elasticity estimates for PERC and METH are positive, showing movements of price and use that are contrary to expectation. I believe the complexity of these two markets make the separation of price effects from regulatory effects much more difficult to obtain in the aggregate models presented here. The next subsection addresses the issue of what further information is needed to obtain more accurate estimates of price effects in these complicated markets.

Evaluation of Model Estimates

Many of the problems with the estimates for the system of equations that compose the chlorinated solvents model stem from shortcomings in the available data. In the PERC equation, no relative price effect could be estimated for the dry cleaning sector because no measures could be found to represent the prices of substitutes to dry cleaning. Many of the small uses for the other chemicals were also excluded due to an absence of appropriate data.

Even when many different sectors can be modeled, the magnitude of the coefficients on the various sectors can be questioned. The METH equation, for instance, suggests that metal cleaning is almost as

¹²Following the notation of the previous footnote the implied sector elasticity is:

$$\epsilon_{y,X} = \frac{\partial y}{\partial X} \cdot \frac{X}{y} = \left[\beta + \alpha \left(\frac{P_{own}}{P_{sub}} \right) \right] \cdot \frac{X}{y}$$

Table 7
PRICE ELASTICITY ESTIMATES

Chemical	Mean Price Elasticity	Standard Error
PERC	.1717	.0951
METH	.7067	.3886
TCE	- .2216	.1280
TCA	- .8296	.1555

important an end use as CFC-11 substitute uses (foam blowing and aerosol applications). This is simply untrue. The culprit in this case is, I argue, the lack of sufficient independent variation in the various sector and price measures. Technically this condition is known as multicollinearity and it implies that sound estimates of the independent effects can not be arrived at. The prediction from the equation will be unbiased, but the model will not be able to separate out the independent effects in its parameter estimates.¹³

To get around the problem of multicollinearity, one needs additional information. For the case of chlorinated solvents, independent measures of the amount of chemical used in each end use are

¹³The magnitude of this problem can be measured by collinearity diagnostics. Following the methods of Belsley, Kuh, and Welsch (1982), condition indices and the variance decompositions of the data matrix associated with each of the four equations were computed using the Singular Value Decomposition. The data for the METH market, in particular, exhibited extremely poor conditioning (the last two condition indices were well over one thousand.) The other equations would often show one eigenvector capturing high proportions of the variance of both the index of industrial activity and the associated interaction term. For cases involving extreme collinearity, the method of principle components or biased estimation (such as James-Stein estimators) can be attempted to improve precision of the parameter estimates. Alternatively, one can try to find better conditioned data.

needed. Though these data are not regularly published by the government, *a priori* estimates are available on an irregular basis. Trade journals, such as the *Chemical Marketing Reporter*, publish estimates every few years of the share of total production taken by a particular end use. In order to assay the plausibility of price and sector effects, another approach was tried that used this *a priori* information.

Available share estimates were used to generate estimates of the amount of solvent consumed by each end use--i.e., the total production value was multiplied by the share estimate. Since the share estimates are made on a less than annual basis, the missing values were interpolated. Naturally, this severely restricts the inference that can be formally made from these data. Because the share estimates are themselves interpolated, statistical inference based upon the data they generate will be completely conditional on the validity of the share estimates. This exercise is, nevertheless, followed through to demonstrate the approach and to give an estimate of market effects *in the absence* of collinearity among end uses¹⁴.

This exercise uses estimates of the amount of each chemical used in each end use in simple models generated by the following equation:

$$\text{Share Quantity} = \beta_0 + \beta_1 X + \alpha_1 [X (P/P)] + \tau_1 [X \text{ Trend}]$$

Since the left hand variable is entirely constructed, no complicated error structure will be specified. The estimation method of ordinary least squares, though no less arbitrary than any other method, is simple and easy to understand. Table 8 shows the coefficient estimates analogous to the complete model; it specifies a single equation for each end use, using the constructed end use share of total production quantity described above. All of the coefficients agree with *a priori*

¹⁴If this information can be obtained at a later point in time, this approach could be followed to produce results that could sustain rigorous statistical inference.

Table 8
COMPLETE MODEL ON CONSTRUCTED END USE SHARE QUANTITIES
OLS SINGLE EQUATION ESTIMATES

Chemical	End Use	Coefficient Estimates (Students' t in parentheses)			
		Constant β_0	Index β_1	Rel. Price α_1	Trend τ_1
PERC					
	METDX	-14778.26 (-9.71)	316.23 (14.13)	-84.17 (-5.86)	
	KNITS	43004.88 (13.91)	153.50 (4.12)		-21.46 (-10.50)
METH					
	METDX	5036.00 (1.64)	-22.06 (-0.42)	36.41 (1.54)	
	FBLOW	-10291.11 (-4.71)	317.30 (6.70)	-83.61 (-1.29)	
	PAINT	10600.38 (2.35)	96.40 (1.36)	-11.23 (-0.68)	
TCE					
	METDX	19393.78 (2.13)	626.43 (5.10)	-229.40 (-3.25)	-39.62 (-11.82)
TCA					
	METDX	-20171.50 (-2.10)	984.21 (6.35)	-250.05 (-3.89)	-.30 (-0.09)

expectations, with the sole exception of METH used in metal cleaning end uses. (Even here, the coefficients do not have a high level of significance.) The mean price elasticity estimates are negative and reasonable, as is shown by Table 9. They suggest that almost all end uses demonstrate sensitivity to changes in the market price of a solvent relative to substitute solvents--substitution matters. These estimates

should not be taken literally, of course; most hinge on fewer than ten actual (estimated share) data points. Nonetheless, the parameter estimates seem less convoluted when the appropriate data are available to eliminate the noise from collinearity among end use measures.

Table 9

PRICE ELASTICITY ESTIMATES FROM CONSTRUCTED END USE MODELS
OLS SINGLE EQUATION ESTIMATES

Chemical	End Use	Mean Price Elasticity	Standard Error
PERC			
	METDX	-.7609	.1299
METH			
	METDX	.5486	.3557
	FBLOW	-.2450	.1897
	PAINT	-.1587	.2309
TCE			
	METDX	-.4008	.1231
TCA			
	METDX	-.7311	.1876

IMPLICATIONS FOR REGULATORY POLICY

I argue that for the difficult case I have selected--the interrelated markets for chlorinated solvents--limitations of the available data create severe statistical problems. After discussing the resulting qualifications I need to make about the individual estimates from the chlorinated solvents model, I address broader questions. How can this type of model show the effect of market substitution in response to regulation? And, more generally, what are policy analytic uses of this type of model that can be used to make informed regulatory policy?

Qualifications

The model of chlorinated solvents presented in this paper generates estimates of price and sector parameters of uneven quality. The equations for simple markets, such as TCE and TCA markets with one predominate end use, generate believable parameter estimates. The equations for the more complex markets, such as PERC and METH, simply do not produce satisfactory parameter estimates for their many end uses. Improved data on these markets would be necessary to generate parameter estimates reliable enough for applications in regulatory analysis. Based upon the current work, however, the model of chlorinated solvents can still explicate important lessons for future statistical research of other chemical markets.

The major limitations of the statistical methods presented thus far are directly tied to the quality and quantity of the data. First, no direct measure was found to characterize regulation. Though deterministic functions of time can be estimated as proxies for regulatory effects, the statistical inference from a formal model will be limited by the accuracy of the estimated proxy. Second, many markets will have substitute chemicals that are either difficult to define or difficult to find accurate measures for. Effects omitted from a model due to lack of suitable data will induce bias in the estimates of remaining effects. Last, data are not readily available on the amount

of chlorinated solvent used in each end use. Where these data are unavailable, models of aggregate use will be limited by the correlation among supposedly independent effects. For chemical markets with many end uses, aggregate use data may not contain sufficient independent variation to separate out the independent effects within each end use.

Applications: Modeling the Effect of Market Substitution

The type of model pioneered in this paper can vividly show the effect of market substitution in response to government regulation. One powerful way to demonstrate this market response, uses the model to simulate the system-wide effect of placing regulations on an individual chemical. Simulating the effect of regulation uses the following logic. A regulatory control placed on a chemical imposes additional costs upon the users of that chemical. This can be thought of as an incremental increase in the effective price of using that chemical. When users face a higher price for one chemical, they will use less of that chemical by finding a cheaper substitute.

The model can demonstrate the consequence of this substitution among chemicals through simulation. Model simulation can be thought of as the inverse of model estimation. When a model is estimated, the data are taken as given. Estimates of the model parameters are generated so as to "fit" the data. When this estimated model is used to simulate an outcome, the reverse occurs. The simulation treats the estimated sector and price parameters in a model as given and allows the data to take on other values.

I show the effect of regulation by adding the increase in the effective price, ΔP , to the existing price P . The new price, $P + \Delta P$, replaces the old price at the point in time the regulation occurs. Using this altered price data, an estimated model will generate a different prediction of chemical use. In our case, the increase in the effective price of the regulated chemical will translate into a lower level of predicted use of that chemical.

To work through an example using the estimated chlorinated solvents model, assume that in 1980 the EPA required new controls for TCE uses in metal cleaning. These regulatory controls were costly, increasing the effective price of TCE use by fifty percent, i.e., $\Delta P = .50 * P$. Figure 8 shows the effect of this regulation by generating one set of predictions using the unaltered price of TCE (P) and another set of predictions using the altered price of TCE ($P' = P + \Delta P = 1.5 * P$). The predicted use of TCE goes down after the regulation, with TCA increasing as users substitute for the relatively cheaper solvent.

Further applications of this type of model in policy analysis of regulatory policy include estimating changes in user surplus, estimating parameters for cost benefit analysis, and predicting the likely effects of new solvent conserving technologies. However, in order to have confidence in the estimates generated by these applications, more robust model estimates would be necessary. This requires improved data on the amount of chemical used by each end use. Given these data, robust model estimates could be obtained and used in these applications to improve regulatory analysis.

Coda: Policy Analysis and Regulatory Policy

It should be noted, strictly speaking, that this research is not a "Policy Analysis". It does not attempt to encompass the entire range of alternative policies concerning the regulation of toxic substances. It is, however, a hard look at one ingredient in a policy analysis of toxic substance regulation--the role and function of economic markets. Analysis of regulatory policy has all too often overlooked the response of economic forces to government regulation. This research establishes not only that this interaction exists, but can be measured and incorporated into the analysis of the consequences of alternative regulatory policies. It is hoped that the analytic approach put forward by this dissertation will contribute to the goal of more rigorous policy analysis and, ultimately, better choices among difficult policy alternatives.

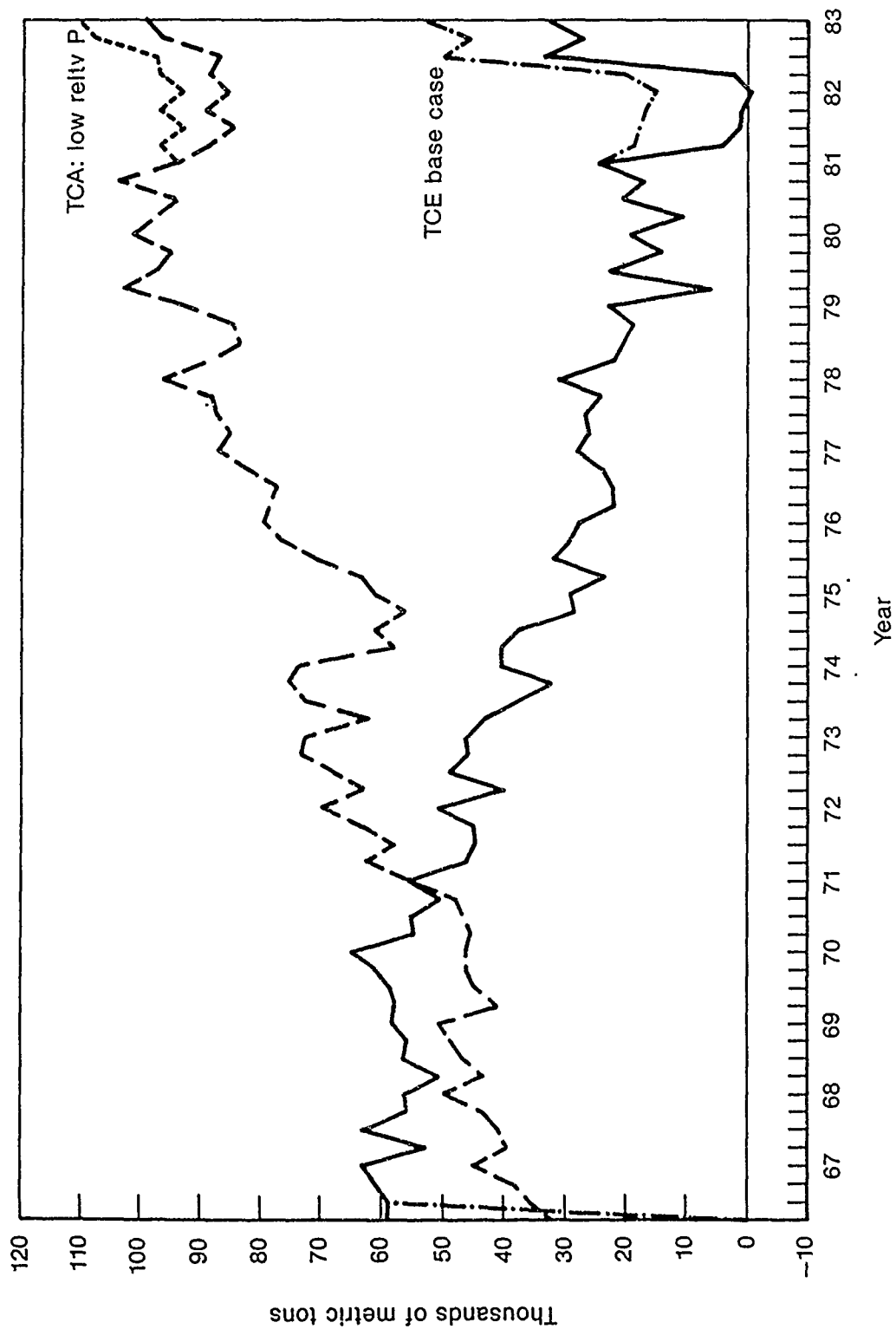


Fig. 8—Simulation of regulation as a cost (1980, cost of using TCE increases 50%)

V. CONCLUSION

The main conclusion of this research is that substitution among potentially toxic chemicals is important in considering a regulatory approach. The chlorinated solvents are an excellent example of a set of widely used interrelated chemicals. They are substitutes for one another in a variety of applications; one of them is used to produce another; some are coproducts in production processes; groups of them are regulated under the same statutes; and they all pose a serious, but different, potential threat to human health. As EPA contemplates the form of future regulations, it is clear that the solvents must be considered together.

The technical analysis lays the base for the empirical analysis and stresses several points. First, the knowledge of the chemicals and their production technology and costs allows one to construct measures of changing marginal feedstock costs over time. These in turn aid identification in the empirical analysis of how solvent price affects solvent use. Second, a good knowledge of the current and historical markets for the chlorinated solvents is essential in analysis of potential regulation. Not only do chlorinated solvents interact in a myriad of end uses, they have undergone considerable regulatory scrutiny over time. An understanding of these regulatory events is a necessary underpinning to a formal model of chlorinated solvent use.

The empirical analysis sought to measure the important relationships set forth in the technical analysis. First, intervention analysis documented the powerful effect of regulation upon the markets for chlorinated solvents--had no regulatory intervention occurred, the use of some solvents would have been much higher. Next a systemwide model of the chlorinated solvents markets, using time proxies for regulatory effects, showed the need to incorporate measures of regulation in this type of empirical modeling. Further analysis of this model, particularly when compared with *a priori* information, pointed to problems inherent in the available data that limit the statistical

inference the model would support. These qualifications are discussed as well as possible applications in the policy analysis of regulatory policy.

The historical approach, incorporating both a technical analysis and an empirical analysis, can be used to examine the effect of regulation on markets for chlorinated solvents. A formal method for handling these market linkages is necessary to understand the implicit risk tradeoffs brought about when markets substitute among chemicals in the presence of regulation. In the future, the types of models presented herein should be used to analyze proposed regulatory alternatives.

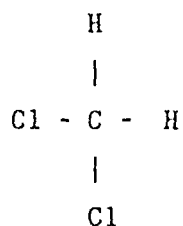
APPENDIX A: CHEMICAL STRUCTURE AND PRODUCTION TECHNOLOGY

Appendix A: Chemical Structure and Production Technology

Chemical Structure

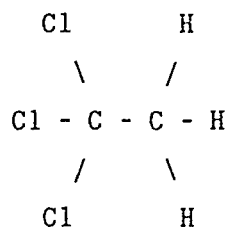
The chemical structure and chemical properties of the chlorinated solvents will be discussed prior to the production technology.

METH, an unsaturated aliphatic compound, has the molecular formula $C H_2 Cl_2$ and the structural formula:



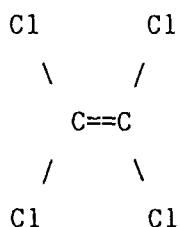
The molecular weight is 84.94, and the composition in percent by weight is: 14.14% C, 2.37% H, and 83.49% Cl. METH is a colorless nonflammable liquid with a mild ethereal odor. It is slightly soluble in water and completely miscible with other chlorinated solvents, diethyl ether, and ethyl alcohol. It dissolves most other organic solvents and is an excellent solvent for many resins, waxes, and fats. It is also one of the more stable chlorinated solvents.

TCA, a saturated aliphatic compound, has the molecular formula $C_2 H_3 Cl_3$ and the structural formula:



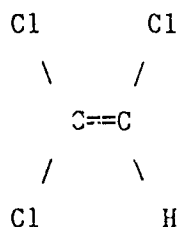
The molecular weight is 133.42, and the composition in percent by weight is: 18.00% C, 2.27% H, and 79.72% Cl. TCA is colorless nonflammable volatile liquid with an ethereal odor and low solubility in water. It is soluble in acetone, benzene, carbon tetrachloride, methanol, and ether.

PERC, an unsaturated aliphatic compound, has the molecular formula $C_2 Cl_4$ and the structural formula:



The molecular weight is 165.85, and the composition in percent by weight is: 14.48% C and 85.52% Cl. PERC is a clear colorless nonflammable liquid with a pleasant ethereal odor. It has substantial vapor pressure and a low solubility in water. It dissolves sulfur, iodine, mercuric chloride, and aluminum chloride. It is the most stable of the chlorinated ethanes and ethylenes, requiring only small amounts of stabilizers.

TCE, an unsaturated aliphatic compound, has the molecular formula C_2HCl_3 and the structural formula:



The molecular weight is 131.40, and the composition in percent by weight is: 18.28% C, 0.77% H, and 80.95% Cl. TCE is a nonflammable liquid with sweet odor resembling chloroform. It is practically insoluble in water and is miscible with ether, alcohol, and chloroform. The nonflammability and volatility make this a very useful solvent.

Production Technology

The major chemical reactions used to manufacture chlorinated solvents are chlorination, hydrochlorination, dehydrochlorination, and oxychlorination. A chlorination reaction substitutes or adds chlorine into the hydrocarbon molecule. Hydrochlorination reactions add chlorine by using hydrogen chloride; dehydrochlorination reactions reverse the procedure by splitting out hydrogen chloride from a chlorinated hydrocarbon molecule. Since large amounts of hydrogen chloride are formed as by-products the ability to economically use the by-product often determines the economic feasibility of the chlorination process. This has led to the development of oxychlorination reactions that combine the hydrogen chloride with an oxidant in the presence of a catalyst to produce other valuable products.

In general, progressive substitution of chlorine atoms for hydrogen atoms lowers the vapor pressure, reduces the flammability, increases the density and viscosity, and modifies the solvent power. Specific heat, water solubility, and dielectric constant vary inversely with chlorine content. All of these characteristics control the unusual properties that make the chlorinated solvents commercially important.

METH: The two predominant methods to produce METH use methane (natural gas) or methanol. The direct reaction of methane with chlorine at high temperatures yields METH and several other chlorinated coproducts. A hydrochlorination reaction combines methanol with hydrogen chloride with the aid of a catalyst to give methyl chloride; this is then chlorinated to produce METH.

TCA: Most TCA comes from a hydrochlorination reaction of vinyl chloride that yields 1,1-dichloroethane; this is then thermally or photochemically chlorinated to produce TCA. Another process adds hydrogen chloride to vinylidene chloride (1,1-dichloroethylene) in the presence of a catalyst to yield TCA.

PERC: For many years most PERC was manufactured in acetylene processes, with TCE as a coproduct. Due to the high cost of acetylene, most PERC now derives from reactions using propane or ethylene dichloride (EDC) as feedstocks. Propane may be thermally chlorinated to yield PERC and hydrogen chloride. Perc may also be derived by chlorinating or oxychlorinating EDC. The latter yields TCE as a coproduct.

TCE: In the mid sixties, most of the TCE produced in the country came from an acetylene reaction. Acetylene and chlorine are combined in the presence of PERC and antimony trichloride to produce 1,1,2,2-tetrachloroethane. This is dehydrochlorinated to produce TCE and hydrogen chloride.

The amount of TCE produced by the acetylene process began to decline in the late sixties, as reactions based on EDC became more economically feasible. EDC, derived from the chlorination or oxychlorination of ethylene, was itself chlorinated and then dehydrochlorinated to produce TCE. The oxychlorination of EDC using a copper chloride catalyst produces PERC and TCE as coproducts. The PERC and TCF mixture is separated and neutralized with ammonia.

- 76 -

APPENDIX B: QUALITATIVE HISTORY

Appendix B: Qualitative History

Table B.1

PERCHLOROETHYLENE
(PERC)

<u>Year</u>	<u>Event</u>
1953	change in TLV to 200 ppm.
1961	Change in TLV to 100 from 200 ppm.
1966	government procurement leads to ups and downs (erratic) in perc demand.
1967	rapid growth in perc for production of CFC-113 and CFC-114. Tariff Commission for 1959 through 1965 shows 18.4 percent annual growth for CFC- 114. There is a new perc stabilizer that isn't water soluble. Will give longer life.
1968	gain in first quarter attributed to one-shot order by government for large quantity of specially fluorinated cleaning solvents (CFC-11 and CFC-113?).
1973	EPA pressure on other solvents could increase perc's market, but perc will have to compete with other exempt solvents.
1976	perc picked up some demand because of exempt solvent status. EPA regs pulling pressure on other solvents will increase perc's market somewhat.

- 1977 NCI carcinogenicity test, positive in mice; inconclusive in rats.
- 1979 CPSC branded perc a carcinogen.
Petroleum solvent will not replace it because of flammability.
- 1980 an epidemiological study showed some positive cancer.
- 1982/83 dry cleaning machinery more efficient and recycling have cut demand. Use for CFC production continues to grow.
- UNDATED perc is photochemically reactive. Twelve states have general VOC regs which include emissions from metal cleaning.
- 1985 NTP carcinogenicity test finds some evidence in mice and clear evidence in rats.

- Between 1982 and 1984/85, TLV changed to 50 ppm.

Table B.2

TRICHLOROETHYLENE
(TCE)

Year	Event
1961	change of TLV from 200 to 100 ppm.
1964	rising demand; booming auto industry.
1965	TCE demand rising because of aerospace and military demand for degreasing of metal in Vietnam War.
1966	huge growth and capacity taxed because of Vietnam War requirements reflecting back on metal production. TLV revised from 100 and 520 (STEL) to 100 and 535 (STEL).
1968	L.A. County adopted Rule 66 which limits TCE emissions.
1969	strong activity in aircraft, space and other metal industries, but TCE not doing well because of pollution legislation in L.A. County. Private study (SRI for MCA) of TCE effects on atmosphere downgrades TCE role as troublemaker. Sharp disagreement about whether methyl chloroform will take some of TCE market.
1970	TCE holding its own in what industry believes is overzealous antipollution efforts on West Coast.

- 1972 several states now have legislation on air emissions patterned after L.A.'s Rule 66. On the other hand, TCE has not been banned under present air quality plans of other states and municipalities. See no growth.
- 1974 EPA reports similarity in human metabolism for TCE and vinyl chloride (known carcinogen).
- 1975 TCE very photoreactive. Federal and local government have severely restricted use and emissions of TCE in vapor degreasing plants in many areas of the country. Some outright bans (e.g., Rhode Island). TCE must be trapped and recycled.
Evidence that TCE is potent carcinogen.
Substitution from TCE to perc and methyl chloroform being actively pushed by some manufacturers.
NCI memo of alert issued on TCE. Indicates preliminary findings are that it will show carcinogenic activity in mice.
- 1977 conversion away from TCE especially in vapor degreasing.
- 1978 emissions and use of TCE have been restricted by EPA. This cuts demand because it requires recycling or substitution. Expect decline until 1983 when it will level off.
- 1979 TCE placed on notice of intended TLV change.
- 1981 loss of market to other solvents should abate, but aggressive marketing of methyl chloroform could cause more loss in TCE.
Notice of intended change to 50 (TLV) and 270 (STEL) ppm.
- 1983 EPA is still scrutinizing TCE and other solvents will continue to replace it.

Between 1981 and 1984/85, TLV lowered to 50 ppm.

Table B.3

TRICHLOROETHANE
(TCA)

<u>Year</u>	<u>Event</u>
1968	change of TLV to 350 and STEL to 1900 ppm.
1971	not clear if growth retarded by recession.
1974	recovery in growth from 1971. Observe conversion from TCE to methyl chloroform to comply with air pollution standards. Methyl chloroform is exempt from such standards.
1977	conversion from TCE to methyl chloroform especially in vapor degreasing. Conversion from toluene to methyl chloroform because of new regulations on the flammability of adhesive formulations. In latter half of 1976, NIOSH recommended ceiling concentration of 350 ppm for 15 minute exposure saying that there is no evidence that methyl chloroform is carcinogenic. NCI bioassay proved negative, but testing has not been discontinued. OSHA formulating new standards for methyl chloroform which should be ready in mid 1977.
1982/83	methyl chloroform demand hit hard by recession. It is highly dependent on automotive, appliance, and aerospace industries.

Table B.4

METHYLENE CHLORIDE
(METH)

<u>Year</u>	<u>Event</u>
1966	demand boostd by Vietnam War. Growth in methylene chloride started 3 years ago when aerosol makers began converting from CFC to hydrocarbons. Degreasing good in war efforts.
1967	government buying for Vietnam War slumped.
1976	growth good, could get better because of demise of CFC propellants and increasing problems with TCE. Change of TLV from 500 to 200 ppm.
1981	change of TLV from 200 to 100 ppm.
1982	recent NTP test shows clear evidence of carcinogenicity, could hurt coffee decaf industry.
1983	Dow came out with a new methylene chloride-based paint stripper.

Table B.5

GENERAL EVENTS

<u>Year</u>	<u>Event</u>
1966	Increased use of chemical solvents as the level of economic activity increases during the Vietnam War.
1973	Energy crisis disrupts and ultimately restructures feedstock prices. Availability problems with chlorine.
1974	Explosion of Shell ethylene plant in the Netherlands.
mid 1970s	Increased regulation of petrochemical solvents
1978	toxicity problem of chlorinateds not resolved (TCE, perc, and methyl chloroform). Some users investigative alkaline wash systems. In general, vapor degreasing is preferred for small precision parts and nonferrous metals. Alkalines used for large, rough parts.
1979	users continue to shift away from water-based detergents and alkalines.
1981	demand for chlorinateds down (TCE, methyl chloroform) because of economic slowdown, and switch to plastics, and increase in foreign made consumer goods. As yet, regulations are unclear. Modest move away from water.
1984	Congress passes amendments to RCRA banning land disposal of chlorinateds in November of 1986.

APPENDIX C: ANALYSIS OF MARGINAL FEEDSTOCK COSTS

Appendix C: Analysis of Marginal Feedstock Costs

Cost of Production

To understand the economic forces driving the markets for chemical solvents, some account must be made of the effect of changes in the costs of producing the solvents. This section describes how data on the costs of feedstock chemicals may be combined to estimate the marginal feedstock cost for each solvent.

Feedstock Prices

Price data on the chemical solvents are of obvious importance in trying to understand historical market forces. The identification of supply and demand forces through time, however, requires that one control for cost shifts. For example, an increase in the costs of feedstock chemicals will increase the marginal production cost of the resultant chemical. This may be interpreted as an upward shift in the supply function for that chemical, since producers would have to be offered a higher price to maintain the same level of production. It is essential to control for these shifts in the supply curve in order to identify a market demand function. Hence it becomes necessary to obtain measures for the costs of inputs to chemical solvents.

To develop a time series of the material costs of various production processes, monthly bulk prices were collected for the chemical solvents and their feedstocks from the *Chemical Marketing Reporter* (CMR). Estimates for natural gas prices come from the *Monthly Energy Review* and the *Natural Gas Monthly*. Liquid propane prices come from *Platts Oil Price Handbook and Oilmanac*, 61st Edition, 1984. The solvents' prices will be used in the estimation of a market model and their feedstock prices will be used to control for changes in the marginal cost of production. The units on all prices were converted to a dollar price per metric ton.

Because of the units used in the CMR or because of changes in the units used, some standardization of prices was required. In particular, prices listed by volume (gallon) had to be converted to weight (metric tons) using a density coefficient. For example, each gallon of LPG

weighs about 4.88 pounds (-44.5°C). To convert a price given in cents per gallon to dollars per pound, the original price must be divided by 4.88 X 100. This, in turn, must be divided by 2204.62 to give a price in metric tons. The following density coefficients were used:

Chemical	Density	Temperature	Reference
Methanol	.7928 g/ml	20° C	4° C H ₂ O
TCA	1.3249 g/ml	26° C	4° C H ₂ O
Methane	.04885 lb/ft ³	20° C	
LPG	.5853 g/ml	-44.5° C	4° C H ₂ O

Source: *Handbook of Chemistry & Physics*, 52nd Edition, and
Chemical Rubber Company *Handbook of Compressed Gas*,
2nd Edition, Compressed Gas Association.

Input-Output Coefficients

To derive a summary feedstock cost for a production process, one needs to know how many pounds of feedstock are required for one pound of resultant chemical in that particular production process. Table C.1 shows this physical relationship between the production process for a chemical and its feedstocks. Though labeled as "input-output" coefficients, they come directly from the stoichiometric weights in the chemical balance equation describing a particular production process after accounting for production inefficiencies.

To illustrate the derivation, the input-output relationship of the PERC required in the production of CFC-113 may be found by applying the following general formula:

$$\text{I-O coefficient} = \frac{\text{Precursor Molecular Weight}}{\text{Resultant Molecular Weight}} \times \frac{1}{\text{Efficiency}} \times \frac{1}{(1 - \text{Fraction Emitted})}$$

The molecular weight for PERC (C₂Cl₄) is 165.85 and that for CFC-113

Table C.1

INPUT-OUTPUT COEFFICIENTS

END PRODUCT	PERC				TCE			TCA			METH	
	1	2	3	4	1	2	3	1	2	3	1	2
PROCESS =												
FEEDSTOCK CHEMICAL												
Chlorine	.48	.92	3.22	1.08	.26	1.17	1.08	.60	1.60	1.93	.91	
Ethylene Dichloride	.68	.64			.85	.82						
Hydrogen Chloride		-.43	-1.28	-.28		-.86	-.28			-.86	-.83	
Oxygen	.26				.21							
Propane			.27									
Carbon Tet			.90									
Acetylene				.20			.20					
Vinyl Chloride								.53				
Ethane									.22			
Methane										.21		
Methanol											.41	
TOTAL MATERIALS COST												
(Dollars/Pound)	.1226	.1141	.1582	.1529	.1118	.1132	.1551	.1200	.701	.899	.901	
KEY = PERC 1 Oxychlorination of EDC												
2 Chlorination of EDC												
3 From Propane												
4 From Acetylene												
TCE 1 Oxychlorination of EDC												
2 Chlorination of EDC												
3 From Acetylene												
TCA 1 From Vinyl Chloride												
2 From Vinylidene Chloride												
METH 1 Chlorination of Methane												
2 Hydrochlorination of Methanol												

($C_2Cl_3F_3$) is 187.39. The production efficiency of the process used to create CFC-113 (reaction of hydrogen fluoride and chlorine with PERC) has been estimated by industry sources as 0.98 and the fraction emitted has been estimated to be 2 percent. This yields the following calculation.

$$\begin{array}{rclclcl} \text{I-O of PERC} & 165.85 & & 1 & & 1 \\ & \hline \text{into CFC-113 :} & 187.39 & \times & \frac{1}{0.98} & \times & \frac{1}{0.98} & = & 0.92 \end{array}$$

Feedstock Costs

An exploratory static analysis of the importance of various feedstock chemicals in the production of chemical solvents was also undertaken. Table C.2 shows the share of each feedstock cost as a proportion of total material costs. From this, one may see the relative importance of each feedstock within any one manufacturing process.

More important, however, might be the relative importance of the cost of a feedstock to the total production cost of a manufacturing process. One measure of the sensitivity of total production cost to a feedstock cost is an elasticity: It shows the percentage increase in production cost that comes about from a 1 percent increase in the feedstock cost. In the short run where the capital stock is fixed, the elasticity may be calculated by multiplying the share given in Table C.2 by the proportion of total production costs taken up by material costs.¹ Table C.3 shows this calculation for midsized production facilities running at 75 percent of full capacity. The elasticities for material costs in large sized production facilities will be larger, since material costs form a larger proportion of total costs.

Although the static analysis is interesting for understanding the present situation, it will not help for understanding and measuring the historical role of feedstock costs in solvent markets. To generate an

¹This is true because the derivative of total production cost with respect to the cost (price) of a feedstock will reduce to the derivative of total material cost, which is the input-output coefficient. The levels of feedstock price and the total production cost, used to standardize the above slope, may be algebraically juggled to produce the above result.

Table C.2

SHARE OF CHEMICAL COST IN MATERIAL COSTS

END PRODUCT	PERC				TCE			TCA			METH	
	1	2	3	4	1	2	3	1	2	1	2	
PROCESS =												
FEEDSTOCK CHEMICAL												
Chlorine	.26	.54	1.37	.48	.16	.70	.47	.34	1.54	1.45	.68	
Ethylene Dichloride	.59	.59			.80	.77						
Hydrogen Chloride		-.24	-.53	-.12		-.47	-.12		-.80	-.60		
Oxygen	.04				.04							
Propane			.19									
Carbon Tet			-.91									
Acetylene				.57			.57					
Vinyl Chloride								.66	.26			
Ethane										.15		
Methane											.32	
Methanol												
KEY = PERC 1 Oxychlorination of EDC												
	2	Chlorination of EDC						TCA 1	From Vinyl Chloride			
	3	From Propane						2	From Vinyl Chloride			
	4	From Acetylene										
TCE 1 Oxychlorination of EDC												
	2	Chlorination of EDC						METH 1	Chlorination of Methane			
	3	From Acetylene						2	Hydrochlorination of Methanol			

Table C.3
ELASTICITY OF PRODUCTION COST
WITH RESPECT TO FEEDSTOCK COST

END PRODUCT	PERC				TCE			TCA			METH	
	1	2	3	4	1	2	3	1	2	3	1	2
PROCESS =												
FEEDSTOCK CHEMICAL												
Chlorine	.17	.29	.45	.31	.10	.39	.31	.17	.75	.57	.27	
Ethylene Dichloride	.38	.32			.52	.43						
Hydrogen Chloride		-.13	-.17	-.08		-.26	-.08		-.39	-.23		
Oxygen	.03				.03							
Propane			.06									
Carbon Tet			-.30									
Acetylene				.37			.37					
Vinyl Chloride								.32				
Ethane								.13				
Methane									.06			
Methanol											.12	
Fraction of Total Prod. Cost taken by Feedstock Costs	.64	.54	.33	.65	.65	.56	.65	.49	.49	.39	.39	
100 MT Plant 75% Capacity												
KEY =												
PERC 1	Oxychlorination of EDC				TCA 1			From Vinyl Chloride				
2	Chlorination of EDC				2			From Vinyl Chloride				
3	From Propane											
4	From Acetylene											
TCE 1	Oxychlorination of EDC				METH 1			Chlorination of Methane				
2	Chlorination of EDC				2			Hydrochlorination of Methanol				
3	From Acetylene											

estimate of the historical feedstock costs for one process one need only weight the price of the feedstocks by their respective input-output coefficients. To generate the summary measure of feedstock costs for any given chemical, the different processes used to manufacture one chemical must be combined. The equations that generate the measure of feedstock costs--by combining the different manufacturing processes--are given in Table C.4. Rather than assume a constant share for each production process, the equations of Table C.4 use derived estimates for how the process shares vary through time. These share estimates are reported in Table C.5. The summary measure of feedstock costs play an important role in the construction of an empirical model of chlorinated solvents.

Table C.4

MARGINAL FEEDSTOCK COST SERIES
EQUATIONS FOR GENERATING ESTIMATES FOR MARGINAL FEEDSTOCK COSTS

```
*-----MARGINAL FEEDSTOCK COST FOR PERC-----;
PERC_MC = IPD_GNP * (
    P_OXY_SH * ( .48 * CL_P + .68 * EDCL_P )
  + P_CHL_SH * (0.92 * CL_P + .64 * EDCL_P - .43 * HCL_P)
  + P_PRO_SH * (3.22 * CL_P + .27 * PROPAN_P
                - 1.28 * HCL_P - 0.90 * CTT_P)
  + P_ACE_SH * (1.08 * CL_P + .20 * ACTYLN_P - .28 * HCL_P)
);

*-----MARGINAL FEEDSTOCK COST FOR METH-----;
METH_MC = IPD_GNP * (
    M_ANE_SH * (1.93 * CL_P - 0.83 * HCL_P + .21 * NGAS_P)
  + M_NOL_SH * ( .91 * CL_P + .41 * MET_P)
);

*-----MARGINAL FEEDSTOCK COST FOR TCE-----;
TCE_MC = IPD_GNP * (
    E_OXY_SH * ( .26 * CL_P + .85 * EDCL_P )
  + E_CHL_SH * (1.17 * CL_P + .82 * EDCL_P - .81 * HCL_P)
  + E_ACE_SH * (1.08 * CL_P + .20 * ACTYLN_P - .28 * HCL_P)
);

*-----MARGINAL FEEDSTOCK COST FOR TCA-----;
TCA_MC = IPD_GNP * (
    A_VCL_SH * ( .60 * CL_P + .53 * VCL_P )
  + A_ETH_SH * (1.60 * CL_P + .22 * ETHANE_P - 0.86 * HCL_P)
);
```

Note: IPD_GNP is the GNP implicit price deflator.

Table C.5

MARGINAL FEEDSTOCK COST SERIES
ESTIMATES FOR PROCESS SHARE OF TOTAL PRODUCTION

CHEMICAL PROCESS = YEAR	PERC				TCE			TCA		METH	
	OXY 1	CHL 2	PRO 3	ACE 4	OXY 1	CHL 2	ACE 3	VCL 1	ETH 2	ANE 1	NOL 2
65	.008	.110	.625	.257	.005	.145	.850	.900	.100	.500	.500
66	.023	.131	.635	.211	.015	.135	.850	.900	.100	.500	.500
67	.039	.151	.645	.165	.035	.215	.750	.900	.100	.479	.532
68	.054	.172	.655	.119	.065	.335	.600	.900	.100	.436	.574
69	.070	.192	.665	.073	.090	.380	.530	.900	.100	.394	.617
70	.085	.200	.665	.050	.100	.390	.510	.900	.100	.351	.659
71	.100	.195	.655	.050	.135	.535	.330	.900	.100	.314	.694
72	.116	.194	.645	.045	.215	.650	.135	.900	.100	.282	.726
73	.131	.196	.635	.038	.300	.590	.110	.900	.100	.250	.758
74	.147	.196	.625	.033	.379	.530	.092	.900	.100	.218	.790
75	.162	.185	.623	.030	.429	.495	.391	.905	.095	.186	.822
76	.173	.174	.628	.025	.455	.485	.375	.915	.085	.170	.830
77	.180	.172	.633	.015	.485	.475	.040	.908	.092	.170	.830
78	.187	.171	.638	.005	.515	.463	.020	.884	.116	.175	.823
79	.198	.175	.627	.000	.545	.448	.005	.860	.140	.170	.835
80	.215	.185	.600	.000	.565	.435	.000	.836	.164	.150	.855
81	.232	.195	.573	.000	.575	.425	.000	.812	.188	.130	.875
82	.248	.205	.547	.000	.588	.413	.000	.800	.200	.110	.895
83	.265	.215	.520	.000	.603	.398	.000	.800	.200	.090	.915
84	.282	.225	.493	.000	.618	.383	.000	.800	.200	.070	.935
85	.290	.230	.480	.000	.625	.375	.000	.800	.200	.060	.940

APPENDIX D: SPECIFICATION OF THE ERROR STRUCTURE

Appendix D: Specification of the Error Structure

The following assumptions are made about the error term:

First-order autocorrelation: $e_{it} = \rho_{ii}e_{i,t-1} + \varepsilon_{it}$

Zero Mean: $E(\varepsilon_{it}) = 0$ for all i, t .

Homoskedastic variance: $E(\varepsilon_{it}, \varepsilon_{jt}) = \sigma_{ij}$ for all i, j, t .

Contemporaneous covariance: $\sigma_{ij} \neq 0$ for $i \neq j$.

$$E(\varepsilon_i, \varepsilon'_j) = \sigma_{ij} I_T \text{ and } E(\varepsilon, \varepsilon') = \Sigma \quad I_T$$

where

$$\begin{matrix} \Sigma = \\ (M \times M) \end{matrix} \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} \end{bmatrix}$$

The complete covariance matrix $E(ee') = \Omega$ is more complicated, but need not be specified to estimate the β and α . The generalized least squares (GLS) estimator of β can be obtained from

$$\beta = (Z' \Omega^{-1} Z)^{-1} Z' \Omega^{-1} y \quad (3.1)$$

Since Ω is unknown, however, an estimate for Ω must be substituted. It will be computationally convenient to find a transformation matrix R such that

$$R \Omega R' = \Sigma \otimes I \quad (3.2)$$

This implies that $\Omega^{-1} = R' (\Sigma^{-1} \otimes I) R$ and that equation 3.1 can be

rewritten

$$\beta = (Z^* (\Sigma^{-1} \otimes I_T) Z^*)^{-1} Z^* (\Sigma^{-1} \otimes I_T) y^* \quad (3.3)$$

Where $Z^* = RZ$ and $y^* = Ry$ are the observations transformed with the

matrix R . The assumption of stationary covariances for the e_{it} 's requires that special treatment be made for the first observation in each equation since it will depend on the values of the first observations in all the other equations. Alternatively, a less cumbersome procedure is to drop the first observation in the transformation. This approximate estimator has the same asymptotic properties but loses efficiency by dropping $M=4$ observations. The transformation matrix R that satisfies (3.2) is a block diagonal matrix:

$$R_{M(T-1) \times MT} = \begin{bmatrix} R_{11} & 0 & 0 & 0 \\ 0 & R_{22} & 0 & 0 \\ 0 & 0 & R_{33} & 0 \\ 0 & 0 & 0 & R_{44} \end{bmatrix}$$

where

$$R_{ii}^{(T-1) \times T} = \begin{bmatrix} -\rho_{ii} & 1 & 0 & \dots & 0 \\ 0 & -\rho_{ii} & 1 & \dots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

In finite samples, the approximate transformation matrix will not necessarily lead to less a efficient estimator (Doran and Griffiths, 1983).

When the elements Σ_{ij} and ρ_{ii} are replaced by their estimates $\hat{\sigma}_{ij}$ and $\hat{\rho}_{ii}$, the GLS estimator becomes an approximate estimated general least squares (EGLS) estimator.

The estimation for chlorinated solvent use proceeds in the following steps.

1. Obtain estimates for the values of the relative price interaction terms from the instrumental equation containing the marginal feedstock costs. Substitute the predicted values for the price terms into Z .
2. Estimate $\hat{\rho}_{ii}$ from the second stage least square (2SLS) on solvent use:

$$\hat{\rho}_{ii} = \frac{\sum_{t=2}^T e_{it} e_{i,t-1}}{\sum_{t=2}^T e_{i,t-1}^2}$$

3. Use the estimated values of ρ for the estimated transformation matrix R . Then transform the observations, $Z^* = R Z$ and $y^* = R y$.

4. Apply Seemingly Unrelated Regression (SUR) to the transformed observations to obtain the estimate for the covariance matrix, Σ , and thence the EGLS estimator:

$$\beta = (Z^* (\Sigma^{-1} \otimes I_{T-1}) Z^*)^{-1} Z^* (\Sigma^{-1} \otimes I_{T-1}) y^*$$

APPENDIX E: SAMPLE SAS PROGRAM
APPROXIMATE GLS - SEEMINGLY UNRELATED REGRESSION WITH AR(1)
CORRECTION

Appendix E: Sample SAS Program Approximate GLS - Seemingly Unrelated Regression with AR(1) Correction

```

*-----BEGIN MODEL STATEMENT-----;
PROC MODEL OUT=RHO_SUR LIST;
  ENDOGENOUS
    PERC_PU
    MET_PRP
    METH_PU
    MET_MRP PAI_MRP FBL_MRP
    TCE_PU
    MET_ERP
    TCA_RU
    MET_ARP ;
  EXOGENOUS  METDX PMETDX MMETDX EMETDX AMETDX
    BLSDX KNITS PAINT FLOW
    PERC_MC METH_MC TCE_MC TCA_MC F11_MC LPG_P
    Q1 Q2 Q3;
  PARAMETERS
    BOP  B1P  B2P  B3P
        A1P
    CO   C1   C2   C3
        C4   C5   C6
        T11P T12P T13P

    BOM  B1M  B2M  B3M
        A1M  A2M  A3M
        T11M T12M T13M
    EO   E1   E2   E3
        E6   E7   E8
        E11  E12  E13
    FO   F1   F2   F3
        F6   F7
        F11  F12  F13
    GO   G1   G2   G3
        G6   G7
        G11  G12  G13

    BOE  B1E
        A1E
    JO   J1   J2   J3
        T11E T12E T13E

    BOA  B1A
        A1A
    KO   K1   K2   K3
        T11A T12A T13A
    ;

```

LABEL

B0P = 'PERC -- INTERCEPT, UNSPECIFIED USE'
B1P = 'PERC -- METAL CLEANING INDEX'
B2P = 'PERC -- DRY CLEANING INDEX'
B3P = 'PERC -- KNIT GARMENTS'
A1P = 'PERC -- INTERACTION OF METDX*P_AE_SP'
T11P= 'PERC -- WINTER QTR DUMMY'
T12P= 'PERC -- SPRING QTR DUMMY'
T13P= 'PERC -- SUMMER QTR DUMMY'
C0 = 'MET_PRP INSTRUMENT, INTERCEPT'
C1 = 'MET_PRP INSTRUMENT, METDX'
C2 = 'MET_PRP INSTRUMENT, BLSDX'
C3 = 'MET_PRP INSTRUMENT, KNITS'
C4 = 'MET_PRP INSTRUMENT, PERC_MC'
C5 = 'MET_PRP INSTRUMENT, TCA_MC'
C6 = 'MET_PRP INSTRUMENT, TCE_MC'
C11 = 'MET_PRP INSTRUMENT, Q1'
C12 = 'MET_PRP INSTRUMENT, Q2'
C13 = 'MET_PRP INSTRUMENT, Q3'
B0M = 'METH -- INTERCEPT, UNSPECIFIED USE'
B1M = 'METH -- METAL CLEANING INDEX'
B2M = 'METH -- PAINTS'
B3M = 'METH -- AEROSOL PROXY, METAL CANS'
B4M = 'METH -- URETHANE FOAM, RAND EST.'
A1M = 'METH -- INTERACTION OF METDX*M_AE_P'
A2M = 'METH -- INTERACTION OF PAINT*M_LPG_P'
A3M = 'METH -- INTERACTION OF FBLOW*M_F11_P'
T11M= 'METH -- WINTER QTR DUMMY'
T12M= 'METH -- SPRING QTR DUMMY'
T13M= 'METH -- SUMMER QTR DUMMY'
E0 = 'MET_MRP INSTRUMENT, INTERCEPT'
E1 = 'MET_MRP INSTRUMENT, METDX'
E2 = 'MET_MRP INSTRUMENT, PAINT'
E3 = 'MET_MRP INSTRUMENT, FBLOW'
E6 = 'MET_MRP INSTRUMENT, METH_MC'
E7 = 'MET_MRP INSTRUMENT, TCA_MC'
E8 = 'MET_MRP INSTRUMENT, TCE_MC'
E11 = 'MET_MRP INSTRUMENT, Q1'
E12 = 'MET_MRP INSTRUMENT, Q2'
E13 = 'MET_MRP INSTRUMENT, Q3'
F0 = 'PAI_MRP INSTRUMENT, INTERCEPT'
F1 = 'PAI_MRP INSTRUMENT, METDX'
F2 = 'PAI_MRP INSTRUMENT, PAINT'
F3 = 'PAI_MRP INSTRUMENT, FBLOW'
F6 = 'PAI_MRP INSTRUMENT, METH_MC'
F7 = 'PAI_MRP INSTRUMENT, LPG_P'
F11 = 'PAI_MRP INSTRUMENT, Q1'
F12 = 'PAI_MRP INSTRUMENT, Q2'
F13 = 'PAI_MRP INSTRUMENT, Q3'
G0 = 'FBL_MRP INSTRUMENT, INTERCEPT'
G1 = 'FBL_MRP INSTRUMENT, METDX'

```

G2 = 'FBL_MRP INSTRUMENT, PAINT'
G3 = 'FBL_MRP INSTRUMENT, FBLOW'
G6 = 'FBL_MRP INSTRUMENT, METH_MC'
G7 = 'FBL_MRP INSTRUMENT, F11_MC'
G11 = 'FBL_MRP INSTRUMENT, Q1'
G12 = 'FBL_MRP INSTRUMENT, Q2'
G13 = 'FBL_MRP INSTRUMENT, Q3'
BOE = 'TCE -- INTERCEPT, UNSPECIFIED USE'
B1E = 'TCE -- METAL CLEANING INDEX'
A1E = 'TCE -- INTERACTION OF METDX*E_A_P'
T11E = 'TCE -- WINTER QTR DUMMY'
T12E = 'TCE -- SPRING QTR DUMMY'
T13E = 'TCE -- SUMMER QTR DUMMY'
J0 = 'MET_ERP INSTRUMENT, INTERCEPT'
J1 = 'MET_ERP INSTRUMENT, METDX'
J2 = 'MET_ERP INSTRUMENT, TCE_MC'
J3 = 'MET_ERP INSTRUMENT, TCA_MC'
BOA = 'TCA -- INTERCEPT, UNSPECIFIED USE'
B1A = 'TCA -- METAL CLEANING INDEX'
A1A = 'TCA -- INTERACTION OF METDX*A_E_P'
T11A = 'TCA -- WINTER QTR DUMMY'
T12A = 'TCA -- SPRING QTR DUMMY'
T13A = 'TCA -- SUMMER QTR DUMMY'
K0 = 'MET_ARP INSTRUMENT, INTERCEPT'
K1 = 'MET_ARP INSTRUMENT, METDX'
K2 = 'MET_ARP INSTRUMENT, TCA_MC'
K3 = 'MET_ARP INSTRUMENT, TCE_MC'
;
MET_PRP = C0 + C1*METDX + C2*BLSDX + C3*KNITS
          + C4*PERC_MC + C5*TCE_MC + C6*TCA_MC ;
PERC_PU = B0P + B1P*PMETDX + B2P*BLSDX + B3P*KNITS
          + A1P*MET_PRP
          + T11P*Q1 + T12P*Q2 + T13P*Q3 ;

MET_MRP = E0 + E1*METDX + E2*PAINT + E3*FBLOW
          + E6*METH_MC + E7*TCA_MC + E8*TCE_MC
          + E11*Q1 + E12*Q2 + E13*Q3 ;
PAI_MRP = F0 + F1*METDX + F2*PAINT + F3*FBLOW
          + F6*METH_MC + F7*LPG_P
          + F11*Q1 + F12*Q2 + F13*Q3 ;
FBL_MRP = G0 + G1*METDX + G2*PAINT + G3*FBLOW
          + G6*METH_MC + G7*F11_MC
          + G11*Q1 + G12*Q2 + G13*Q3 ;
METH_PU = B0M + B1M*MMETDX + B2M*PAINT + B3M*FBLOW
          + A1M*MET_MRP+ A2M*PAI_MRP+ A3M*FBL_MRP
          + T11M*Q1 + T12M*Q2 + T13M*Q3 ;

MET_ERP = J0 + J1*METDX + J2*TCE_MC + J3*TCA_MC ;
TCE_PU = BOE + (B1E*EMETDX )
          + (A1E*MET_ERP)
          + T11E*Q1 + T12E*Q2 + T13E*Q3 ;

```

```
MET_ARP = KO + K1*METDX + K2*TCA_MC + K3*TCE_MC ;
TCA_RU = BOA + (B1A*AMETDX )
          + (A1A*MET_ARP)
          + T11A*Q1 + T12A*Q2 + T13A*Q3 ;

*-----END MODEL STATEMENT-----;

*-----ESTIMATE 2SLS-----;
PROC SYSNLIN DATA=CHEM MODEL=RHO_SUR
  2SLS DW
  OUT=RES_2SLS OUTRESID OUTPREDICT;
TITLE 'TOXSYS3G -- SIMULTANEOUS EQ W AR(1) -- 67 TO 83' ;
TITLE2 '-----MULTIPLE EQUATIONS, 3SLS-----' ;
  ID DATE;

*-----PICK OUT PREDICTIONS AND RESIDUALS FROM 2SLS-----;
PROC SORT DATA=RES_2SLS; BY DATE;
DATA TEMP;
  SET RES_2SLS;
  BY DATE;
  RETAIN PRES MRES ERES ARES
        PHAT MHAT MPHAT MFHAT EHAT AHAT
        P_ELAGE P_EE
        M_ELAGE M_EE
        E_ELAGE E_EF
        A_ELAGE A_EE;
  IF _TYPE_ = 'RESIDUAL' THEN PRES=PERC_PU;
  IF _TYPE_ = 'RESIDUAL' THEN MRES=METH_PU;
  IF _TYPE_ = 'RESIDUAL' THEN ERES=TCE_PU;
  IF _TYPE_ = 'RESIDUAL' THEN ARES=TCA_RU;
  IF _TYPE_ = 'PREDICT' THEN PHAT =MET_PRP;
  IF _TYPE_ = 'PREDICT' THEN MHAT =MET_MRP;
  IF _TYPE_ = 'PREDICT' THEN MPHAT=PAI_MRP;
  IF _TYPE_ = 'PREDICT' THEN MFHAT=FBL_MRP;
  IF _TYPE_ = 'PREDICT' THEN EHAT =MET_ERP;
  IF _TYPE_ = 'PREDICT' THEN AHAT =MET_ARP;
  IF LAST.DATE THEN DO;
    MET_PRP = PHAT ;
    MET_MRP = MHAT ;
    PAI_MRP = MPHAT ;
    FBL_MRP = MFHAT ;
    MET_ERP = EHAT ;
    MET_ARP = AHAT ;
  OUTPUT;
  END;
  P_ELAGE = PRES * LAG( PRES ); P_EE = (LAG( PRES))**2;
  M_ELAGE = MRES * LAG( MRES ); M_EE = (LAG( MRES))**2;
  E_ELAGE = ERES * LAG( ERES ); E_EE = (LAG( ERES))**2;
  A_ELAGE = ARES * LAG( ARES ); A_EE = (LAG( ARES))**2;
```



```

*-----ESTIMATE RHO'S FROM 2SLS-----;
DATA RESID (KEEP= P_ELAGE P_EE
              M_ELAGE M_EE
              E_ELAGE E_EE
              A_ELAGE A_EE);

SET TEMP;
  IF _TYPE_ = 'PREDICT' THEN DELETE;
  IF _TYPE_ = 'ACTUAL' THEN DELETE;
  IF _N_=1 THEN P_EE = . ; IF _N_=1 THEN M_EE = . ;
  IF _N_=1 THEN E_EE = . ; IF _N_=1 THEN A_EE = . ;
PROC SUMMARY DATA=RESID;
  VAR      P_ELAGE P_EE
           M_ELAGE M_EE
           E_ELAGE E_EE
           A_ELAGE A_EE;
  OUTPUT OUT=TEMP2 SUM = SP_ELAGE SP_EE
                        SM_ELAGE SM_EE
                        SE_ELAGE SE_EE
                        SA_ELAGE SA_EE;

DATA RHO;
  SET TEMP2;
  PERC_RHO = SP_ELAGE / SP_EE ;
  METH_RHO = SM_ELAGE / SM_EE ;
  TCE_RHO  = SE_ELAGE / SE_EE ;
  TCA_RHO  = SA_ELAGE / SA_EE ;
  MATCH = 100;
PROC PRINT DATA=RHO;
  VAR PERC_RHO METH_RHO TCE_RHO TCA_RHO;
  TITLE 'ESTIMATES OF FIRST ORDER AUTOCORRELATION, RHO';

*-----PICK OUT INSTRUMENT PREDICTIONS FROM 2SLS-----;
DATA TEMP3 (DROP = MET_PRP MET_MRP PAI_MRP FBL_MRP MET_ERP MET_ARP);
  SET CHEM2;
DATA TEMP4 (KEEP = DATE MET_PRP MET_MRP PAI_MRP FBL_MRP MET_ERP MET_ARP);
  SET TEMP;
  IF _TYPE_ = 'RESIDUAL' THEN DELETE;
  IF _TYPE_ = 'ACTUAL' THEN DELETE;
DATA Z;
  MERGE TEMP3 TEMP4;
  BY DATE;

*-----CREATE TRANSFORMED MATRIX FOR GLS ESTIMATION-----;
DATA Z_STAR;
  MERGE Z RHO;
  BY MATCH;
  PERC_PU = PERC_PU - PERC_RHO*LAG(PERC_PU);
  PMETDX  = PMETDX  - PERC_RHO*LAG(PMETDX );
  MET_PRP = MET_PRP - PERC_RHO*LAG(MET_PRP);
  BLSDX   = BLSDX   - PERC_RHO*LAG(BLSDX );
  KNITS    = KNITS   - PERC_RHO*LAG(KNITS );

```

```

METH_PU = METH_PU - METH_RHO*LAG(METH_PU);
MMETDX = MMETDX - METH_RHO*LAG(MMETDX );
MET_MRP = MET_MRP - METH_RHO*LAG(MET_MRP);
PAINT = PAINT - METH_RHO*LAG(PAINT );
PAI_MRP = PAI_MRP - METH_RHO*LAG(PAI_MRP);
FBLOW = FBLOW - METH_RHO*LAG(FBLOW );
FBL_MRP = FBL_MRP - METH_RHO*LAG(FBL_MRP);

TCE_PU = TCE_PU - TCE_RHO *LAG(TCE_PU );
EMETDX = EMETDX - TCE_RHO *LAG(EMETDX );
MET_ERP = MET_ERP - TCE_RHO *LAG(MET_ERP);

TCA_RU = TCA_RU - TCA_RHO *LAG(TCA_RU );
AMETDX = AMETDX - TCA_RHO *LAG(AMETDX );
MET_ARP = MET_ARP - TCA_RHO *LAG(MET_ARP);

*-----ESTIMATE SUR ON TRANSFORMED Z_STAR-----;
PROC SYNLIN DATA=Z_STAR MODEL=RHO_SUR
SUR DW
OUT=PLOTS OUTRESID OUTPREDICT OUTACTUAL;
TITLE 'TOXSYS3G -- SIMULTANEOUS EQ W AR(1) -- 67 TO 83' ;
ID DATE;
FIT PERC_PU METH_PU TCE_PU TCA_RU;

PROC SORT DATA=PLOTS; BY DATE;
DATA PLOTS2;
SET PLOTS;
BY DATE;
RETAIN
PER_PU PHAT PRES
MET_PU MHAT MRES
TE_PU EHAT ERES
TA_PU AHAT ARES;
IF _TYPE_ = 'ACTUAL' THEN PER_PU=PERC_PU;
IF _TYPE_ = 'PREDICT' THEN PHAT=PERC_PU;
IF _TYPE_ = 'RESIDUAL' THEN PRES=PERC_PU;
IF _TYPE_ = 'ACTUAL' THEN MET_PU=METH_PU;
IF _TYPE_ = 'PREDICT' THEN MHAT=METH_PU;
IF _TYPE_ = 'RESIDUAL' THEN MRES=METH_PU;
IF _TYPE_ = 'ACTUAL' THEN TE_PU=TCE_PU;
IF _TYPE_ = 'PREDICT' THEN EHAT=TCE_PU;
IF _TYPE_ = 'RESIDUAL' THEN ERES=TCE_PU;
IF _TYPE_ = 'ACTUAL' THEN TA_PU=TCA_RU;
IF _TYPE_ = 'PREDICT' THEN AHAT=TCA_RU;
IF _TYPE_ = 'RESIDUAL' THEN ARES=TCA_RU;
IF LAST.DATE THEN DO;
PERC_PU=PER_PU;
METH_PU=MET_PU;
TCE_PU=TE_PU;
TCA_RU=TA_PU;
OUTPUT;

```

```
      END;  
PROC PLOT DATA=POUTT2;  
  PLOT PERC_PU*DATE PHAT*DATE='*' /OVERLAY;  
  PLOT PRES*PHAT/ VREF=0;  
  PLOT PRES*DATE/ VREF=0;  
  PLOT METH_PU*DATE MHAT*DATE='*' /OVERLAY;  
  PLOT MRES*MHAT/ VREF=0;  
  PLOT MRES*DATE/ VREF=0;  
  PLOT TCE_PU*DATE EHAT*DATE='*' /OVERLAY;  
  PLOT ERES*EHAT/ VREF=0;  
  PLOT ERES*DATE/ VREF=0;  
  PLOT TCA_RU*DATE AHAT*DATE='*' /OVERLAY;  
  PLOT ARES*AHAT/ VREF=0;  
  PLOT ARES*DATE/ VREF=0;
```

APPENDIX F: THE FUNCTIONAL FORM OF A PROXY FOR REGULATORY
PRESSURE

Appendix F: The Functional Form of a Proxy for Regulatory Pressure Theory

Time trends are typically specified as a constant-slope linear trend through time, implying the effect of regulation increases constantly through time. More realistically, one might expect the effect of regulation to approach a maximum value. If so, a nonlinear time trend would better represent the time effect of regulation. Figure F.1 compares a linear function of time with two nonlinear functions of time: the natural log of time and the square root of time. Either specification represents an improvement over the constant slope of a linear trend term.

The potential advantage of a maximum asymptote may not be sufficient for the case of TCE where regulatory action started slowly at first, in a few limited areas. Gradually regulatory pressure picked up as TCE came under scrutiny for possible toxic effects as well as for photoreactivity. Thus one needs a more flexible proxy through time that can capture the slow initial growth of regulation in addition to an ultimate leveling off at a high level of regulatory pressure.

One candidate for a more flexible function uses a logistic specification:

$$R = \frac{A}{1 + B e^{-C t}}$$

Conveniently the parameters of the logistic function--shown in Fig. F.2--have a readily understandable interpretation that will help in imposing reasonable *a priori* information to aid the estimation process. The scaling parameter A is the maximum value that regulatory pressure may attain and C is the rate of growth of the regulatory pressure. From the first derivative,

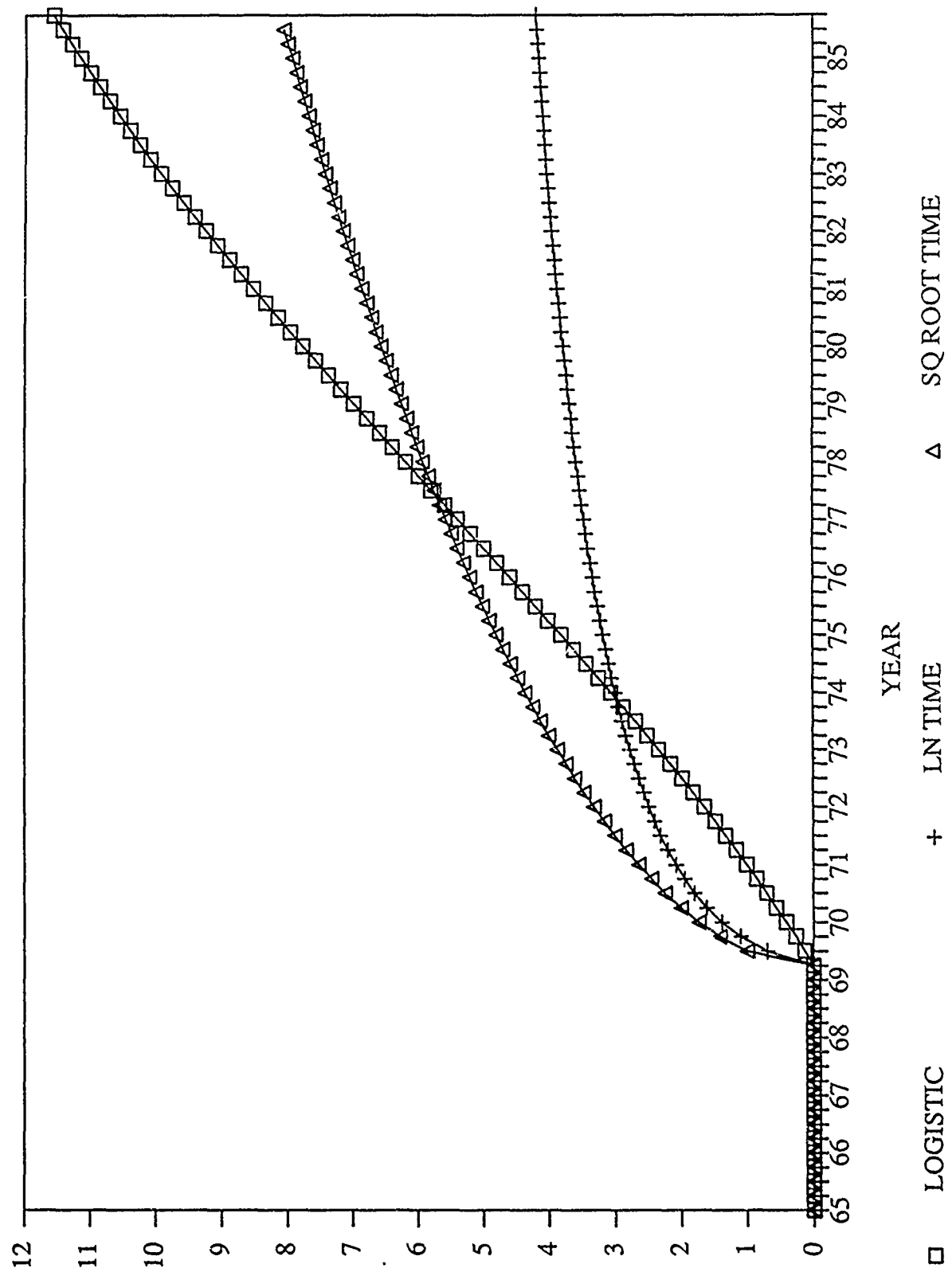
$$\frac{dR}{dt} = \frac{C}{A} R (A - R)$$

it may be seen that the rate of change of R with respect to time is

Dynamic Proxies for Regulatory Pressure

Figure F.1:

Dynamic Proxies for Regulatory Pressure



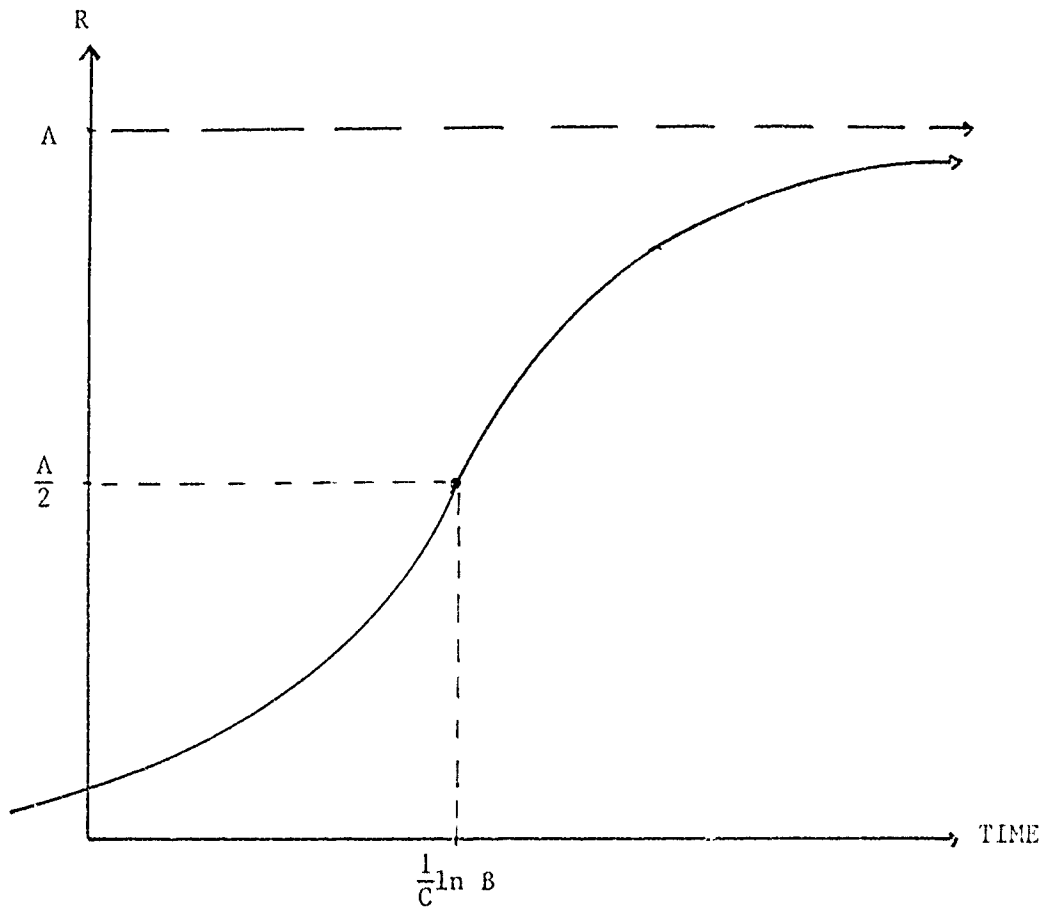


Fig. F.2 The Logistic Function

proportional to the current level of R and to the distance yet to travel to the maximum value "A." The logistic curve is frequently used to represent growth, where growth is thought to be positively related to the existing level and negatively related to the current distance from a maximum level. Set the second derivative,

$$\frac{d^2R}{dt^2} = \frac{C}{A} (A - 2R) \frac{dR}{dt}$$

to zero, to find the inflection point at

$$R = \frac{A}{2}, \quad t = \frac{1}{C} \ln B.$$

The interpretation of the parameters can help specify a proxy for regulatory pressure. If the inflection point were itself an object of interest, in addition to the maximum value and rate of growth of regulation, it may be made more explicit by setting the value of time at the point of inflection equal to I and rewriting the logistic function.

$$R = \frac{A}{1 + e^{\frac{C(I-t)}{A}}}; \quad \text{where } I = \frac{1}{C} \ln B.$$

From this expression one could obtain a proxy for regulatory pressure by imposing *a priori* estimates of the maximum value, the rate of growth, and the inflection point, and then substituting the proxy into the original model to see if it improved the fit of the model. Alternatively, the entire logistic function for the proxy could itself be inserted into the original linear model to make for a nonlinear model where estimates are obtained for one or more of the logistic parameters.

Fitting such a model requires maximizing a nonlinear likelihood function and can be computationally treacherous. The use of outside information on the nonlinear parameters can help control the estimation process. Even if one were to form a grid of possible values of A, C,

and I and compare the mean squared error from each possible model, some bound would have to be placed on the values over which A, C, and I could range. Using outside information, one can reasonably place bounds on the allowable range.

The comparison of the different proxies for regulatory pressure in the case of TCE follows.

Comparison of Results for TCE

The TCE market model illustrated above will serve as the basis for the comparison of the proxies for regulatory pressure. Table F.1 shows a comparison of models using the time proxies that can be expressed in a linear form. A first glance reveals that all the time proxies improve fit, but based solely upon the mean squared error the simple (quarterly) time trend does better than the two incorporating an upper asymptote. The poor performance of both the natural log and the square root of time may be understood in that they imply that the rate of growth of regulation starts out a high level and then gradually slows down. This is contrary to the belief that regulation started slowly and gradually grew.

As a reasonable value for inflection a point three years after the start of regulatory activity in mid-1968 was chosen. Fig. F.3 shows the shape of logistic functions having an inflection point of three years, where the growth rate is allowed to vary. For a completely *a priori* comparison, a model was estimated using the above inflection point and a growth rate of 10 percent. Table F.2 shows a comparison of the *a priori* logistic proxy and the trend proxy. The *a priori* model is somewhat better in terms of fit, but an even greater advantage emerges in the comparison of predictions. The market model using a time trend, shown in Fig. F.4, actually suggest a negative use of TCE by 1980. The predictions from the *a priori* logistic proxy level off in Fig. F.5 and, though they are somewhat too low, come closer to the actual values.

As a test on the information imposed upon the logistic proxy, the models were reestimated over the entire time period. With the additional data, the growth rate was estimated as a parameter. Table

Table F.1

COMPARISON OF LINEAR TREND PROXIES
MARKET MODEL: 1965-1975

VARIABLE	LS	TIME	NAT. LOG TIME	SQ. ROOT TIME	VARIABLE LABEL
INTERCEP	113865.60 (25551.20)	57235.70 (13237.49)	87368.75 (16997.25)	83196.06 (15762.55)	Intercept
METDX	-1886.61 (1647.85)	-1930.85 (794.40)	-4259.82 (1117.76)	-4142.52 (1024.40)	Metal Cleaning Index, SIC 252, 34, 35, 36, 39
MET_ARP	1481.63 (1771.42)	2598.10 (859.29)	5103.93 (1249.08)	5031.65 (1141.93)	Interaction of METDX*(TCA_SP/TCE_SP)
TIME		-1386.07 (118.67)			Linear Time Trend
LN_TIME			-8846.70 (1173.91)		Natural Log of Time
SQRTTIME				-6324.80 (737.34)	Square Root of Time
ROOT MEAN SQ. ERROR	10814.60	5213.60	7038.71	6497.80	
R-SQUARE	0.15	0.81	0.65	0.70	
D.F.	41	40	40	40	

Note: Standard errors are in parentheses.

Logistic Functions: Constant Inflection Point, Growth Rate Varies

Figure F.3:

Dynamic Proxies for Regulatory Pressure

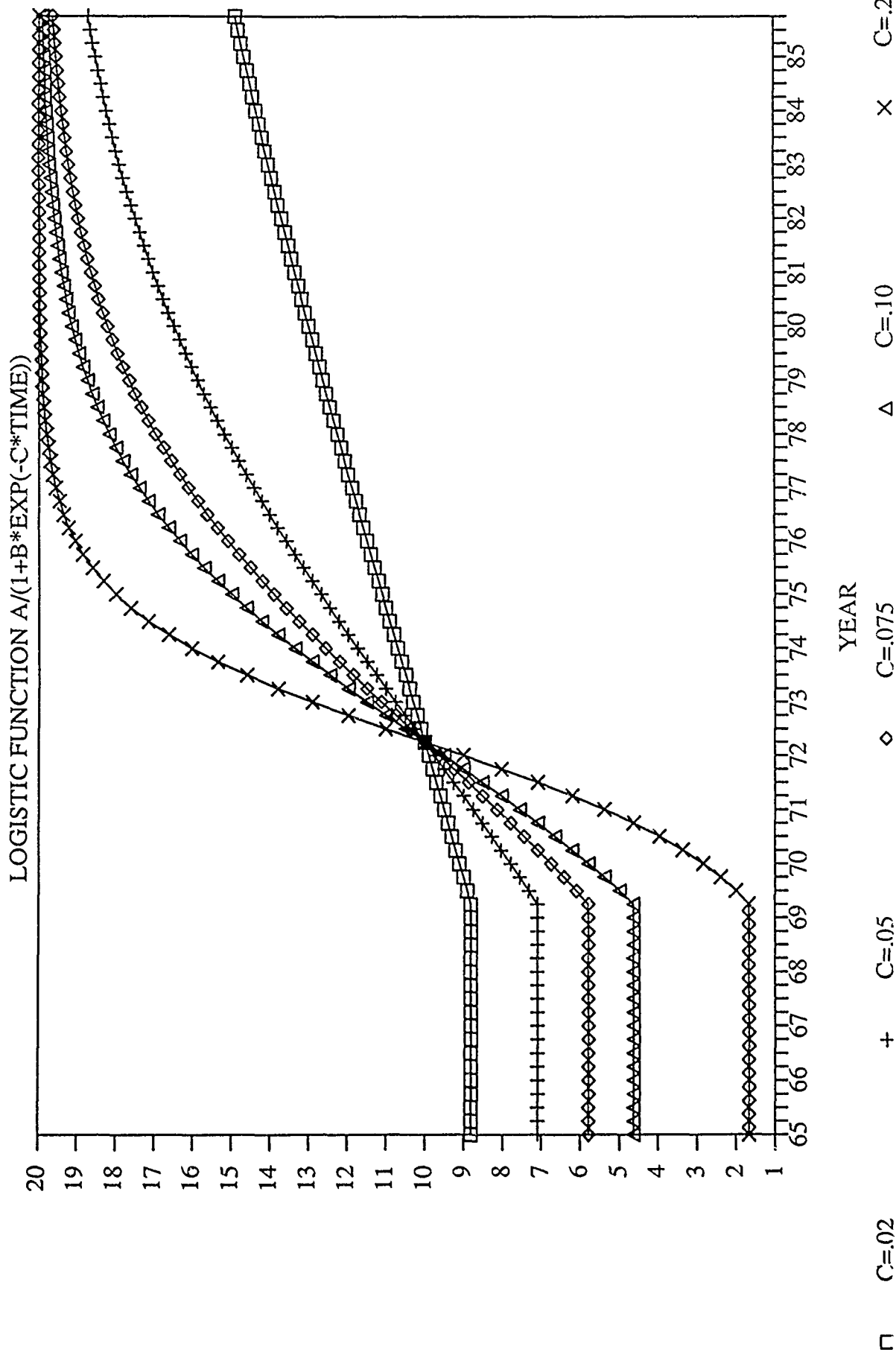


Table F.2

COMPARISON OF LINEAR AND NONLINEAR TIME PROXIES
MARKET MODEL: 1965-1975

VARIABLE	LS	TIME	A PRIORI LOGISTIC	VARIABLE LABEL
INTERCEP	113865.60 (25551.20)	57235.70 (13237.49)	53144.66 (13186.15)	Intercept
METDX	-1886.61 (1647.85)	-1930.85 (794.40)	-1786.46 (783.19)	Metal Cleaning Index, SIC 252, 34, 35, 36, 39
MET_ARP	1481.63 (1771.42)	2598.10 (859.29)	2479.80 (845.85)	Interaction of METDX*(TCA_SP/TCE_SP)
TIME		-1386.07 (118.67)		Linear Time Trend
MAX_A			-62264.08 (5238.07)	Maximum value of Logistic Function
ROOT MEAN SQ. ERROR	10814.60	5213.60	5143.17	
D.F.	41	40	40	

Note: Standard errors are in parentheses.

PLOT OF TCE PU*DATE
PLOT OF PRED*DATE

LEGEND: A = 1 OBS
SYMBOL USED IS *

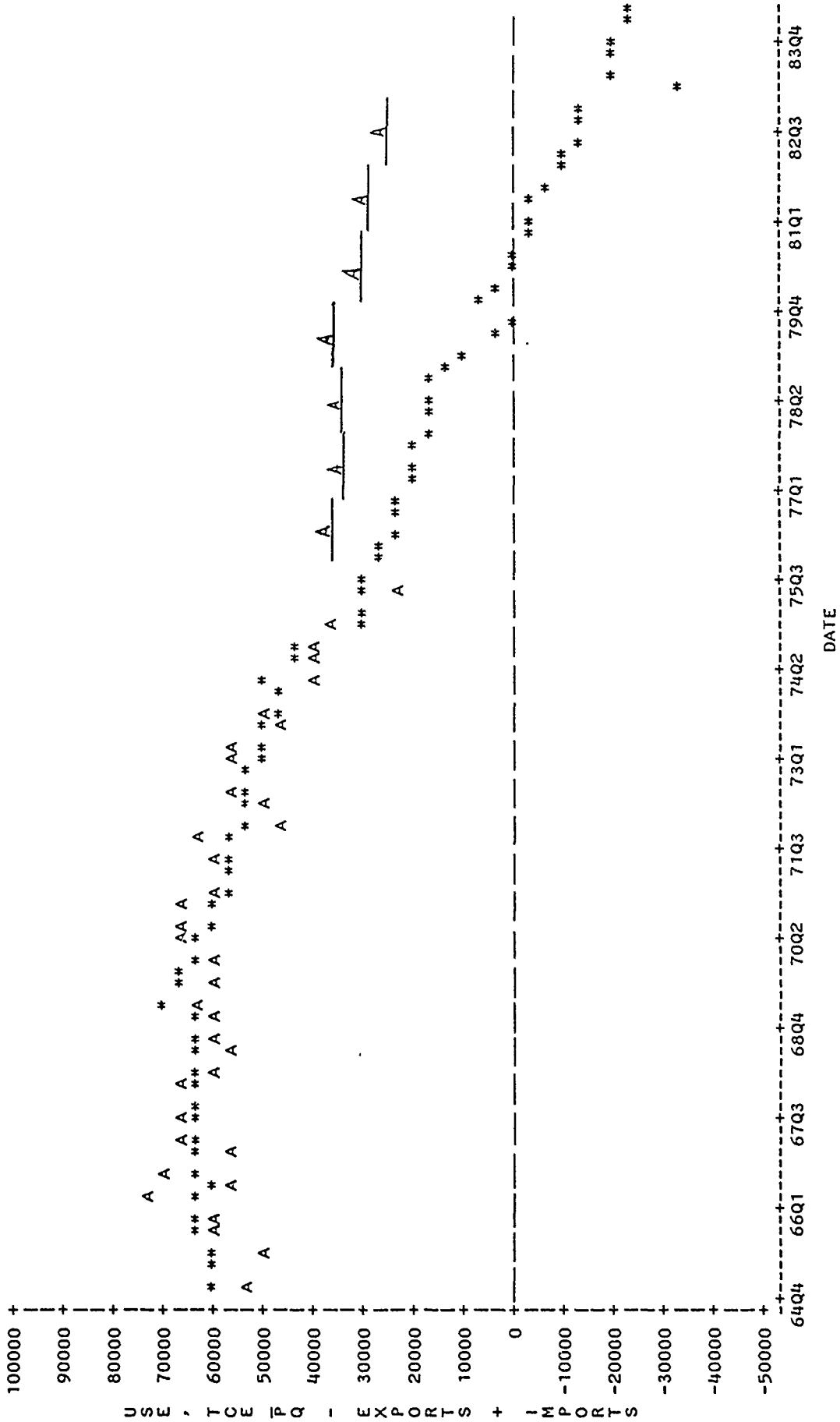


Fig F.4

non-Markov Model with Trend Proxv: Predictions versus Actual

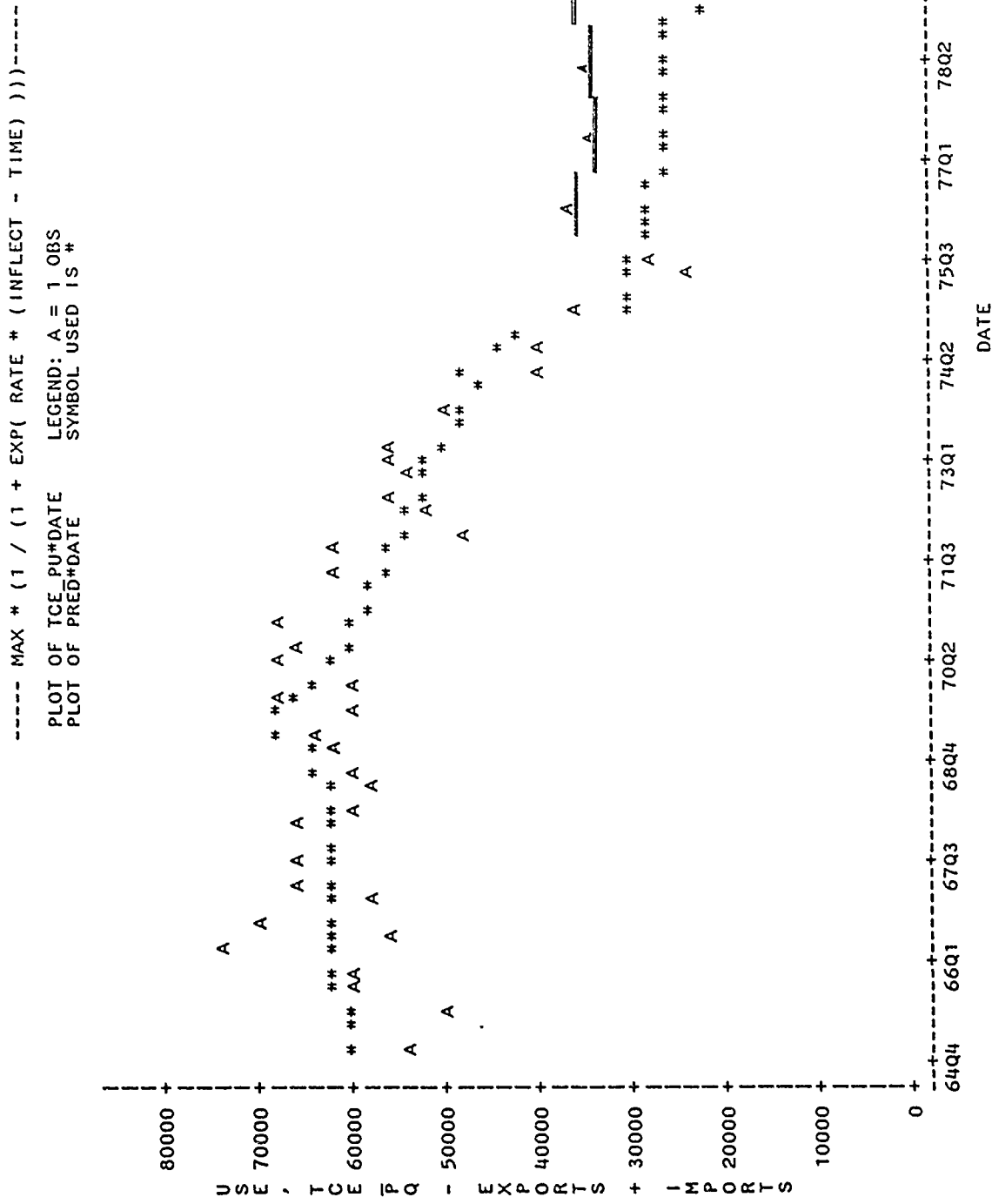


Fig F.5

TCE Market Model with a priori Logistic Proxy: Predictions versus Actual

Table F.3

TCE COMPLETE MODEL: LOGISTIC PROXY WITH ESTIMATED RATE
ENTIRE TIME PERIOD: 1965-1983

VARIABLE	TIME	A PRIORI LOGISTIC	VARIABLE LABEL
INTERCEP	53826.91 (13237.49)	41633.08 (9065.52)	Intercept
METDX	-417.85 (294.20)	298.26 (118.54)	Metal Cleaning Index, SIC 252, 34, 35, 36, 39
MET_ERP	720.46 (318.47)	0 (constrained)	Interaction of METDX*(TCE_SP/TCA_SP)
TIME	- 933.62 (89.55)		Linear Time Trend
MAX_A		-69867.92 (23753.52)	Maximum value of Logistic Function
RATE		0.0829 (0.0310)	Growth Rate of Logistic Function
ROOT MEAN SQ. ERROR	6698.40	5747.95	
D.F.	68	68	

Note: Standard errors are in parentheses, those for the nonlinear logistic model are asymptotic estimates.

F.3 compares the results of the two models estimated over the entire period. The logistic proxy is again better in terms of fit and the estimated value for the growth rate of regulation is about 8 percent, very close to our original *a priori* value.

Obviously the logistic proxy could be fine tuned beyond what is presented here. It is not a perfect proxy but certainly an improvement over a time trend--both in terms of fit and predictive ability. One could hold the rate constant and obtain an estimate for the time value

of the inflection point. One may theoretically estimate all parameters simultaneously, although this sometimes presents computational problems such as ending up on local maximum points on the likelihood surface. A step beyond this would map the likelihood hyperplane and bound the range of rates and inflection points that generate very similar models in terms of fit. Lest the major point be obscured, the judicious use of outside information on the inflection point or growth rate can aid in arriving at a reasonable proxy for regulatory pressure.

REFERENCES

1. American Conference of Governmental Industrial Hygienists, "Threshold Limit Values - Discussion and Thirty-Five Year Index With Recommendations," M.E. Lanier, Ed., Cincinnati, Ohio, 1984.
2. Box, G. E. P., and G. C. Tiao, "A Change in Level of a Non-stationary Time Series," *Biometrika*, Vol 52, June 1965, pp. 181-192.
3. Box, G. E. P., and G. C. Taio, *Bayesian Inference in Statistical Analysis*, Reading, Massachusetts: Addison-Wesley Publishing Co., 1973.
4. Breusch, T.S., and A.R. Pagan, "A Simple Test for Heteroscedasticity and Random Coefficient Variation," *Econometrica*, Vol. 47, 1979, pp. 1287-1294.
5. Brockwell, P. J., and R. A. Davis, *Time Series: Theory and Methods*, New York, Springer-Verlag, 1987.
6. Camm, F., T.H. Quinn, A. Bamezai, J.K. Hammitt, M. Meltzer, W.E. Mooz, and K.A. Wolf, "Social Cost of Technical Control Options to Reduce the Use of Potential Ozone Depleters in the United States: An Update," The Rand Corporation, N-2440-EPA, May 1986.
7. Camm, F., Kohler, D. F., "Choosing the Transition Policies to Implement the Regulation of Toxic Chemicals," N-2586-EPA, August 1986.
8. Chemical and Engineering News, "Chemicals for Electronics: New Growth in Competitive Field," April 8, 1983.
9. Chemical Marketing Reporter, Chemical Profile, 1,1,1-Trichloroethane, January 22, 1974; January 17, 1977; September 27, 1982; March 28, 1983; January 20, 1986.
10. Chemical Marketing Reporter, Chemical Profile, Fluorocarbons, August 21, 1972; September 1, 1975; August 7, 1978; March 7, 1983; March 10, 1986.
11. Chemical Marketing Reporter, Chemical Profile, Methylene Chloride, February 10, 1986; February 28, 1983; July 12, 1982; August 6, 1979; August 6, 1979; September 20, 1976; November 22, 1973.
12. Chemical Marketing Reporter, Chemical Profile, Perchloroethylene, August 13, 1973; August 9, 1976; June 18, 1979; March 22, 1982; March 14, 1983; February 3, 1986.

13. Chemical Marketing Reporter, Chemical Profile, Trichloroethylene, November 20, 1972; September 22, 1975; June 26, 1978; April 6, 1981; February 14, 1983; January 27, 1986.
14. Chow, G.C., "Tests of Equality between Sets of Coefficients in Two Linear Regressions," *Econometrica*, Vol. 28, 1960, pp.591-605.
15. Conrad, J., ed., *Society, Technology and Risk Assessment*, London, Academic Press, 1980.
16. Conrad, J., "Society and Risk Assessment: An Attempt at Interpretation," in Conrad, ed. *Society Technology and Risk Assessment*, 1980, pp. 241-76.
17. Considine, D. M., *Chemical and Process Technology Encyclopedia*, McGraw-Hill Book Company.
18. Dolgin, E. L., and T. G. Guilbert, *Federal Environmental Law*, St. Paul: West Publishing Co., 1974.
19. Doran H.E. and W.E. Griffiths, "On the Relative Efficiency of Estimators which Include the Initial Observations in the Order Autoregressive Disturbances," *Journal of Econometrics*, Vol. 23, 1983, pp. 165-191.
20. Druley, R. M. and G. L. Ordway, *The Toxic Substances Control Act*, Washington, D.C.: The Bureau of National Affairs, Inc., 1977.
21. Environmental Safety, "America's Toxic Protection Gap: The Collapse of Compliance with the Nation's Toxic Laws," Washington, D.C., July 1984.
22. E.I. DuPont de Nemours and Company, "Information Requested by EPA on Nonaerosol Propellant Uses of Fully Halogenated Halocarbons," Wilmington, Delaware, March 15, 1978.
23. Farhad, N. and L.M. Elkin, "Integrated Solvents Analysis: Production of Fluorocarbons 11 and 12 from Carbon Tetrachloride," SRI International, Menlo Park, California.
24. Frankel, G., The Decline and Fall of the American Way of Regulation-Part II, "The Tragedy of TOSCA: Chemical Poisoning the EPA Can't Control," *Washington Monthly*, Vol. 11, Nos. 5 & 6, July - August 1979., pp. 42-45.
25. Franklin Institute Research Laboratories (FIRL), 1975, Preliminary Study of Selected Potential Environmental Contaminants. EPA-560/2-75-002 (PB-243 910, NTIS), July 1975.

26. Gaynor, K., "The Toxic Substances Control Act: A Regulatory Morass," *Vanderbilt Law Review*, Vol. 30, p. 1149, Nov. 1977.
27. General Accounting Office, *EPA's Efforts to Identify and Control Harmful Chemicals in Use*, GAO/RCED-84-100, United States General Accounting Office, Washington D.C., June 13, 1984a.
28. General Accounting Office, *Assessment of New Chemicals Regulation Under the Toxic Substances Control Act*, GAO/RCED-84-84, United States General Accounting Office, Washington D.C., June 15, 1984b.
29. GCA Corporation, "Preliminary Analysis of Possible Substitutes for 1,1,1- Trichloroethane, Tetrachloroethene, Dichloromethane, Tetrachloromethane, Trichloroethene, and Trichlorotrifluoroethane," GCAI Technology Division, Chapel Hill, North Carolina, May 1983.
30. Glass, G. V., "Estimating the Effects of Intervention into a Nonstationary Time Series," *American Educational Research Journal*, Vol. 9, No. 3, 1972, pp. 463-477.
31. Granger, C.W.J and P. Newbold, *Forecasting Economic Time Series*, Academic Press, 1977.
32. Hammitt, J.K., K.A. Wolf, F. Camm, W.E. Mooz, T.H. Quinn, and A. Bamezai, "Product Uses and Market Trends for Potential Ozone Depleting Substances: 1985-2000," The Rand Corporation, forthcoming.
33. Hausman, J.A., "Specification Tests in Econometrics," *Econometrica*, Vol. 46, No. 6, November 1978, p. 1251-1271.
34. Judge, G.G., W.E. Griffiths, R.C. Hill, H. Lutkepohl, and Tsoung-Chao Lee, *The Theory and Practice of Econometrics*, John Wiley and Sons, 1985.
35. Kates, R. W., "Managing Technological Hazard: Research Needs and Opportunities," University of Colorado, Boulder, 1977.
36. Kaus, R., "How the People Lost Control," *Washington Monthly*, July-August 1979, pp. 34-41.
37. Kempton, M., "EPA and Toxics Research: Hands-Off Back Scratching," *Los Angeles Times*, Vol. 103, Section II, September 14, 1984.
38. Kirk-Othmer, 1985, *Concise Encyclopedia of Chemical Technology*, Interscience Publishers, A Division of John Wiley and Sons, Inc., N.Y.
39. Large, A. J., "Toxic-Waste Fights Start in Laboratories But How Good Are the Testing Methods?", *The Wall Street Journal*, June 21, 1983, p. 60.

40. Lawless, Edward W., M.V. Jones, and R. M. Jones, "Comparative Risk Assessment: Toward an Analytical Framework", Final Report, NSF Grant No. PRA-8018868, Midwest Research Institute.
41. Lowenheim, F.A., and M. K. Moran, 1975, Faith, Keyes, and Clark's Industrial Chemicals, Wiley-Interscience Publication, John Wiley and Sons, Inc., N.Y.
42. Lubasch, A. H., E.P.A., "Bowling to Courts, Sets Toxicity Tests," The New York Times, September 30, 1984, Vol. 134, Section 1, p. 34.
43. Merck Index, 1985, 12th ed., Published by Merck and Company, Inc., Rahway, N.J.
44. Mooz, W.E., S.H. Dole, D.L. Jaquette, W.H. Krase, P.F. Morrison, S.L. Salem, R.G. Salter, and K.A. Wolf, "Technical Options for Reducing Chlorofluorocarbon Emissions," The Rand Corporation, R-2879-EPA, March 1982.
45. National Resources Defense Council vs. Costle (1980), 14ERC (1958), DCSNY (1980).
46. "Navigating the Rough Waters of the Nation's Toxics," Chemical Week, Vol. 135, No. 18, October 31, 1984, pp. 90-94.
47. Nelson, C.R., and H. Kang, "Pitfalls in the Use of Time as an Explanatory Variable in Regression," Journal of Business & Economic Statistics, Vol. 2, No. 1, January 1984, pp. 73-82.
48. North, D. W., "TSCA's Impact on Society and Chemical Industry, (Quantitative Analysis as a Basis for Decisions Under TSCA)," The American Chemical Society, 1983, pp. 180-195.
49. "NRC Panel Finds Woeful Lack In Toxicity Testing of Commercial Chemicals," Research and Development, Vol. 26, No. 5, May 1984, pp. 50.
50. Oil, Paint, and Drug Reporter, Chemical Profile, 1,1,1-Trichloroethane, March 25, 1968; April 26, 1971.
51. Oil, Paint, and Drug Reporter, Chemical Profile, Fluorocarbons, March 9, 1970.
52. Oil, Paint, and Drug Reporter, Chemical Profile, Methylene Chloride, February 8, 1971; November 13, 1967.
53. Oil, Paint, and Drug Reporter, Chemical Profile, Perchloroethylene, November 30, 1970.

54. Oil, Paint, and Drug Reporter, Chemical Profile, Trichloroethylene, June 15, 1964; July 11, 1966; October 6, 1969.
55. Palmer, A.R., W.E. Mooz, T.H. Quinn, and K.A. Wolf, "Economic Implications of Regulating Chlorofluorocarbon Emissions from Nonaerosol Applications," The Rand Corporation, R-2524-EPA, June 1980.
56. Park, R. E. and B. M. Mitchell, "Estimating the Autocorrelated error Model with Trended Data," *Journal of Econometrics*, Vol. 13, 1980, pp. 185-201.
57. Portney, P. R., ed., *U. S. Environmental Policy*, Baltimore: The Johns Hopkins University Press, 1978.
58. Prais, G. J., and C. B. Winsten, Trend Estimators and Serial Correlation, Discussion Paper No. 383, Cowles Commission, Chicago, 1954.
59. "Proposed New Toxic Rules May Require 600,000 Firms to Keep Files 5 to 30 Years," *The Wall Street Journal*, , Volume 103, July 9, 1980, p. 4.
60. Quinn, T.H., K.A. Wolf, W.E. Mooz, J.K. Hammitt, T.W. Chesnutt, and S. Sarma, "Projected Use, Emissions, and Banks of Potential Ozone-Depleting Substances," The Rand Corporation, N-2282-EPA, January 1986.
61. Rowe, W.B. "Government Regulation of Societal Risk," *The George Washington Law Review* 45 951, August 1977.
62. Singh, B., A.L. Nagar, N.K. Choudhry, and B. Raj, "On the Estimation of Structural Change: A Generalization of the Random Coefficients Regression Model," *International Economic Review*, Vol. 17, 1976, pp. 340-361.
63. Swamy, P.A.V.B., "Linear models with random coefficients," in *Frontiers in Econometrics*, Paul Zarembka ed., Academic Press, 1974, pp. 143-168.
64. Tucker, W., "The Chemistry is Getting Better at the EPA," *Fortune*, Vol. 106, No. 6, Sept. 20, 1982, pp. 57-60.
65. The New RCRA, "Hazardous and Solid Waste Amendments of 1984," May 9, 1985.
66. "The Toxic Substances Control Act: Overview and Evaluation," Lyndon B. Johnson School of Public Affairs, The University of Texas at Austin, Policy Research Project Report, Number 50, 1982.

67. United States District Court, Southern District of New York, N.R.D.C. vs. Castle, 1979 Civ. 2411, affidavit of Steven D. Jellinek, July 11, 1979.
68. United States International Trade Commission, Synthetic Organic Chemicals, U.S. Production and Sales, 1974 through 1985.
69. U.S. Congress. House. Committee on Interstate and Foreign Commerce. *Toxic Substances Control Act*, 94th Cong., 1st sess., 1975.
70. U.S. Congress. House. Committee on Interstate and Foreign Commerce. *Toxic Substances Control Act*, 94th Cong., 2nd sess., 1975.
71. U.S. Congress. House Conference Committee. *Toxic Substances Control Act*, 94th Cong., 2nd sess., 1976.
72. U.S. Congress. Senate. Committee on Commerce. *Report on Toxic Substances Control Act*, 92nd Cong., 2nd sess., 1972.
73. U.S. Congress. Senate. Committee on Commerce. *Toxic Substances Control Act*, 94th Cong., 1st sess., pt. 1, 1975.
74. U.S. Congress. Senate. Committee on Commerce. *Toxic Substances Control Act*, 94th Cong., 1st sess., pt. 2, 1975.
75. U.S. Congress. Senate. Conference Committee. *Toxic Substances Control Act*, 94th Cong., 2nd sess., 1976.
76. U.S. Council on Environmental Quality, *Annual Report on Environmental Quality*, (Washington D.C.: U.S. Government Printing Office, 1971).
77. U.S. Council on Environmental Quality, *Toxic Substances*, (Washington, D.C.: U.S. Government Printing Office, 1971).
78. U.S. Tariff Commission, Synthetic Organic Chemicals, U.S. Production and Sales, 1964 through 1973.
79. Wolf, K.A., "Regulating Chlorofluorocarbon Emissions: Effects on Chemical Production," The Rand Corporation, N-1483-EPA, August 1980.
80. Wolf, K. and C. Myers, "Hazardous Waste Management by Small Quantity Generators: Chlorinated Solvents in the Dry Cleaning Industry," The RAND Corporation, R-3505-JMO/RC, June 1987.
81. Wolf, K. and F. Camm, "Policies for Chlorinated Solvent Waste: An Exploratory Application of a Model of Chemical Life Cycles and Interactions," The RAND Corporation, R-3506-JMO/RC, June 1987.

82. Woodhouse, E. J., External Influences on Productivity: EPA's Implementation of TSCA," Policy Studies Review, February 1985, Vol. 4, No. 3, pp. 497-503.
83. Worobec, M. D., "The Toxic Substances Control Act," Defense Law Journal, Volume 34, February 1985, pp. 55-73.